Planes and axes of symmetry in an elastic material

by

Riaz Ahmad Khan



A thesis submitted to the

Centre for Advanced Mathematics and Physics, National University of Sciences and Technology, H-12, Islamabad, Pakistan for the degree of Doctor of Philosophy

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Abstract

Physical properties of elastic and piezoelectric materials are studied by using tensors. It is usual to represent a tensor by a matrix. If a tensor is invariant under rotation about a fixed axis, the matrix representing the tensor commutes with rotation matrix. Therefore these two matrices have common eigenvectors, consequently a knowledge of eigenvectors of the rotation matrix provides us with a fair amount of information about eigenvectors of the tensor. This result is utilized to derive familiar representations of a transversely isotropic tensor of rank 2 and the elasticity tensor possessing tetragonal symmetry. Representation of the elasticity tensor belonging to a particular symmetry class can be achieved in an elegant manner.

In an arbitrary coordinate system, it is not obvious to identify the symmetry class of the elastic materials under debate. In such circumstances Cowin-Mehrabadi Theorem plays a vital role. 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. Necessary and sufficient Conditions are obtained for the identification of an *n*-fold axis of symmetry with $n \ge 3$. The treatment is then generalized to a Cartesian tensor of arbitrary rank and consequently the necessary and sufficient conditions are also found for the existence of a plane of symmetry or an axis of symmetry for a piezoelectric material.

Young's modulus is a material property that describes the stiffness of an elastic material. It is therefore one of the most important properties in engineering design. The familiar representation derived for a transversely isotropic (or hexagonal) material in this thesis is applied to find an expression for Young's modulus and consider its optimum values.

The expression of Young's modulus for a hexagonal material is written in terms of one variable only and hence the problem is solved by a straightforward manner.

Dedicated to

My parents

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Chapter 1

Introduction

Material symmetry of an anisotropic elastic material plays an important role in the theory of linear anisotropic elasticity. The constitutive relation for linear anisotropic elasticity is the generalized Hooke's law which describes the most general linear relationship between stress and strain tensors. The fourth rank elasticity tensor emerges from Hooke's law. Elasticity tensor, in three dimensions, has 81 components. Due to symmetries of stress and strain and the thermodynamic requirement that no work be done by the elastic material in a closed loading cycle, the number of independent components reduces to 21 only. Further reduction of independent components was classically based on the crystallographic considerations [1–4]. It was shown by Huo and Del Piero [5] and S. Forte [6] that symmetry in classical anisotropic elasticity are self contained and are independent of crystallography. P. Chadwick et al. [7] have shown that elastic materials can be divided into eight classes and each class being uniquely characterized by a precise set of planes of mirror symmetry for the given elasticity tensor, see also [2,8].

Lord Kelvin first described the properties of an elastic material in terms of eigenvalues and eigenvectors of the elasticity tensor in the middle of the nineteenth century [9]. However, his description was independently discovered again by Rychlewski [10] and by Mehrabadi and Cowin [11] (also see [12,13]). The main idea of [10,11] is to represent the elasticity tensor c of rank 4 in three dimensions, by a tensor \hat{c} of rank 2 in six dimensions. The formulation of interpreting the eigenvectors of \hat{c} , which are 6×1 column vectors, as tensors of rank 2 in three dimensions has several advantages. One advantage is that the coordinate transformations of elasticity tensor can be achieved using matrix multiplications. This means that standard results of linear algebra become applicable. For example, if a coordinate transform is applied to the elasticity tensor such that the elasticity tensor is invariant under the transformation, then the transformation matrix \hat{Q} must commute with the tensor represented by the 6×6 matrix \hat{c} . Ahmad and Khan have [14] used this fact to create matrix representations for \hat{c} belonging to different symmetry classes. There are many applications of the six dimensional representation of the elasticity tensor (see, for example, [15, 16] and references therein). Blinowski and Ostrowska-Maciejewska have found expressions for the Youngs modulus and Poissons ratio in terms of eigenvalues and eigenvectors of the elasticity tensor in case of orthotropic material [17]. In [18], Mehrabadi et al. have discovered six-dimensional representation of the rotation in terms of the axis of rotation **n** and the angle of rotation θ . Norris [19] has derived the coaxiality condition for the strain energy to be a minimum under a state of uniform stress using this representation.

If the trace and determinant of a second rank tensor in three dimensions both vanish, then it is called *pure shear*. Whereas, an *isochoric* tensor is a second rank traceless tensor. A *pure shear* is also isochoric but the converse is not necessarily true. The properties of pure shear have been discussed by Blinowski and Rychlewski in [20]. They have proved the following result

Theorem 1.1. (Blinowski-Rychlewski Theorem). An elastic material is a symmetric one only if at least two of its proper states are pure shears belonging to some subspace of shears with common direction P_A .

In [21], Ahmad has used the six-dimensional formulation of the elasticity tensor to illuminate the following two interesting properties of elastic materials:

(1) An eigenvector of the elasticity tensor represents a state of stress tensor which is proportional to a strain tensor. The top three components of these tensors represent the normal stresses and strains. Vanishing of the sum of normal strains implies that the rate of change of volume is zero i.e. the strain tensor represents an *isochoric* or an *equivoluminal* state. Ahmad has shown that, for all materials which possess a plane of symmetry, at least two such states of strain exist. This result is less general than Theorem 1.1. However, his method is provides a simple proof of this Theorem. (2) A geometrical argument using the 'law of rational indices' establishes the result that if a crystal possesses an *n*-fold axis of symmetry, A_n , then *n* must be such that $cos(2\pi/n)$ is a rational number [22]. This allows n = 2, 3, 4 and 6 but forbids n = 5. However, this argument does not imply that an arbitrary rotation about the A_6 axis should leave the system invariant. On the other hand, Hermann's Theorem [23] states that if a tensor of rank *r* possesses an axis of symmetry A_p with p > r, then A_p is an axis of isotropy for that tensor. Hermann's proof uses sophisticated mathematics to prove his Theorem. Ahmad gives an elementary proof of the result: \hat{c} can have at most four distinct coaxial planes of symmetry and an *n*-fold axis of symmetry, A_n , with n > 4, must be an axis of isotropy. Also see Slawinski ([24], chapter 5).

Physical properties of anisotropic elastic materials are described by means of tensors such as the dielectric tensor, ε , of rank two, the piezoelectric tensor, e, of rank three and the elasticity tensor, \mathbf{c} , of rank four. Tensors may be represented by matrices [26], for instance, the elastic constants of anisotropic materials are written as 6×6 matrix c [27]. An advantage of representing a symmetric tensor by a symmetric matrix is that classical results of linear algebra become readily available which play a significant role in enriching the theory of tensors. For example, the elastic energy of the material is positive if the 6×6 matrix **c** is positive definite. Similarly eigenvectors play an important role in the necessary and sufficient conditions for the identification of plane of symmetry or an axis of symmetry of an elastic material. Components of these tensors which describes the physical properties of anisotropic elastic materials, 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. The origin of this discussion go back to the problem considered by Cowin and Mehrabadi for identifying the elastic symmetry. For a plane of symmetry, they addressed this problem in [28]. They formulated a simple eigenvalue problem for the determination of normals to the plane of symmetry of an elastic material. Let c_{ijkl} , i, j, k, l = 1, 2, 3 denote components of the elasticity tensor. Cowin and Mehrabadi [28] have proved a theorem called Cowin-Mehrabadi Theorem which is stated as follows:

"A set of necessary and sufficient conditions for a unit vector \mathbf{n} to be a normal to a plane of symmetry is that it should be a common eigenvector of the tensors $U_{ij} = c_{ijkk}$, $V_{ij} = c_{ikjk}$, $W_{ik}(\mathbf{n}) = c_{ijks}n_jn_s$ and $W_{ik}(\mathbf{m}) = c_{ijks}m_jm_s$, where \mathbf{m} is any vector lying in the symmetry plane, summation on the repeated indices is understood and free indices take the values 1, 2, 3".

The four conditions of the Cowin-Mehrabadi Theorem were then modified by Cowin [29] to reduce the conditions to last two conditions only. Ting has provided some generalizations of the Cowin-Mehrabadi Theorem in [30]. Ahmad [31] has proved Cowin-Mehrabadi Theorem for an axis of symmetry. He proved a Theorem having the following statement: *"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 $W_{ik}(\mathbf{p}) = c_{ijks}p_jp_s$ ".

Ahmad [21] has also provided a six dimensional formulation of the Cowin-Mehrabadi Theorem.

As a practical example of the identification of elastic symmetry, Cowin and Mehrabadi considered *bone* as an elastic material in [29]. They applied their methods and numerical algorithm to bone tissues to identify the elastic symmetries of bone. But these methods can be applied to all materials.

This thesis is divided into six chapters. In chapter 2, we have reviewed basics of the theory to be covered in the remainder of this thesis. This chapter contains a brief discussion on tensors, generalized Hooke's law, the elasticity tensor and compliance tensor. The reduction of the number of elastic constants due to material symmetry is explained for isotropic and anisotropic materials clearly. Cowin-Mehrabadi formalism [11] defines a tensor in six dimensions, it has been explained in detail and illustrated by an example too. Cowin-Mehrabadi Theorem has been proved with detailed explanations and the modifications by several researchers is also mentioned in different cases. A suitable explanation of piezoelectric tensor is given and the reduction of its components due to symmetry is dis-

cussed. We also discuss the Young's modulus, which is a material property that describes its stiffness and is therefore one of the most important properties in engineering design.

In chapter 3, we shall make use of a well-known result of linear algebra which states that if two Hermitian matrices commute then they can be simultaneously diagonalized. This means that a set of orthonormal vectors exists, every member of which, is a *common* eigenvector of both matrices. If a tensor is invariant under rotation about a fixed axis and the rotation matrix and the matrix representing the tensor commute then these two matrices have common eigenvectors. Therefore by investigating the eigenvectors of the rotation matrix, we can find the eigenvectors of elasticity tensor too and hence apply this result to derive representations of the elasticity tensors in the form

$$\hat{c} = \sum_{i=1}^{6} \lambda_i E_i \tag{1.1}$$

where E_i are 6×6 matrices with properties

$$E_i E_j = 0, i \neq j$$
$$E_i^2 = E_i,$$
$$\sum_{i=1}^{6} E_i = I.$$

The above representation reduces calculations of powers and inverse of \hat{c} to trivial changes in (1.1). Also it is very useful in finding invariant expressions for engineering constants such as Young's modulus, Poisson's ratio etc.

The above representation has in effect partitioned the elasticity tensor into sets which constitute an associative algebra [32]. Our work also reproduces eigenspaces found by Bona et al. in their characterization of the symmetry classes of elasticity tensors [33,34]. These examples are an indication of the power of Mehrabadi-Cowin formalism [11] to approach classical results from a new perspective.

In chapter 4, we provide simple proofs of the necessary and sufficient conditions for the identification of a plane of symmetry or an axis of symmetry given in Cowin-Mehrabadi Theorem and its special case for axis of symmetry [31] by searching for invariant directions associated with the elasticity tensor. In case of plane of symmetry, such a direction must

be orthogonal to the normal **n** whereas in case of axis of symmetry, it must be parallel to the vector **p**. We generalize this approach to tensors of arbitrary rank and apply it to the third rank piezoelectric tensor to identify the plane of symmetry and do the same for an axis of symmetry of piezoelectric material. We also obtain the conditions for the identification of an *n*-fold axis of symmetry with $n \ge 3$. Some of these results are also illustrated by means of explicit examples. These results are developed and generalized to a tensor of arbitrary rank.

Chapter 5 is devoted to the application of familiar matrix representations obtained for the elasticity tensors in chapter 3. The special case of hexagonal materials is discussed there. By using the representation derived in chapter 3, we compute an expression for the Young's modulus and consider its extreme values. This approach extends to hexagonal materials the results of Norris [35] who considered Poisson's ratio in cubic materials.

In chapter 6, the results developed in this thesis are summarized explicitly.

Chapter 2

Preliminaries

2.1 A short review of tensors

Consider a real vector space V and its elements \mathbf{u} , \mathbf{v} , \mathbf{w} ,... are vectors if they satisfy all the axioms of a vector space. An *n*-dimensional vector space is denoted by V_n . Assume that $\{\mathbf{e}_i\}_{i=1}^n$ and $\{\mathbf{e}'_j\}_{j=1}^n$ are two orthonormal bases in V_n . These bases are related by the following equations

$$e'_j = Q_{ij}e_i \text{ and } e_i = Q_{ji}e'_j$$

$$(2.1)$$

where, the matrix $\mathbf{Q} = [Q_{ij}]$ is the transformation matrix. Since this matrix represents the change of an orthonormal basis and hence it is an orthogonal matrix [36]. So that we can write

$$\mathbf{Q}\mathbf{Q}^T = \mathbf{I}, \ det \ \mathbf{Q} = \pm 1 \ and \ \mathbf{Q}^{-1} = \mathbf{Q}^T$$

where

$$\mathbf{I} = \begin{pmatrix} 1 & 0 & \dots & 0 \\ 0 & 1 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & 1 \end{pmatrix},$$

therefore we have $\mathbf{Q}^{-1} = \mathbf{Q}^T = [Q_{ji}].$

Thus a vector \mathbf{u} can be expressed in two ways

$$\mathbf{u} = u_i e_i$$
 and $\mathbf{u} = u'_j e_j$.

Now using (2.1), we can write the following relations

$$u'_{j} = Q_{ij}u_{i} \text{ and } u_{i} = Q_{ji}u'_{j}.$$
 (2.2)

These relations are called the transformation law of components of a vector. The matrix form of (2.2) is

$$\mathbf{u}' = \mathbf{Q}\mathbf{u}$$
 and $\mathbf{u} = \mathbf{Q}^T\mathbf{u}'$

where, $\mathbf{u} = [u_1, u_2, ..., u_n]^T$ and $\mathbf{u}' = [u_1', u_2', ..., u_n']^T$. This change of basis plays an important role in the theory of material symmetry.

2.1.1 Second order tensor

Let V be a real vector space. A linear function \mathbf{T} defined on V and having values in V is called a *second order tensor* [36]. That is we can write

$$\mathbf{u} = \mathbf{T}(\mathbf{v}) = \mathbf{T}\mathbf{v}, \ \mathbf{u}, \ \mathbf{v} \in V \text{ and}$$
$$\mathbf{T}(\alpha \mathbf{u} + \beta \mathbf{v}) = \alpha \mathbf{T}\mathbf{u} + \beta \mathbf{T}\mathbf{v}, \ \forall \ \mathbf{u}, \ \mathbf{v} \in V, \ \forall \ \alpha, \ \beta \in \mathbb{R}$$

The second order tensors play a fundamental role in the mechanics of deformable bodies because deformation and internal forces characterizing the behaviour of deformable bodies are described mathematically by second order tensors such as strain and stress tensors. The second order tensor satisfy all the axioms of a vector space. We denote the vector space of all second order tensors by \mathcal{L} .

The product $\mathbf{u} \otimes \mathbf{v} = \mathbf{u}\mathbf{v}$ of two vectors $\mathbf{u}, \mathbf{v} \in V$, defined on V and having values in V such that it is a linear function is called *tensor product* or *dyadic product*. That is we can write

$$(\mathbf{u} \otimes \mathbf{v})(\mathbf{w}) = \mathbf{u}\mathbf{v}(\mathbf{w}) = \mathbf{u}(\mathbf{v}.\mathbf{w})$$
, for all $\mathbf{w} \in V$

and

$$\mathbf{uv}(\alpha \mathbf{x} + \beta \mathbf{y}) = \alpha \mathbf{uv}(\mathbf{x}) + \beta \mathbf{uv}(\mathbf{y}), \text{ for all } \mathbf{x}, \mathbf{y} \in V.$$

We note that the tensor product of two vectors \mathbf{u}, \mathbf{v} is also a second order tensor.

Let $\{e_k\}_{k=1}^n$ be an orthonormal basis in V_n . Consider $\mathbf{T} \in \mathcal{L}$ an arbitrary tensor. Thus $\mathbf{T}e_m \in V_n$ can be written as

$$\mathbf{T}e_m = T_{km}e_k$$
, for all $\mathbf{T} \in \mathcal{L}$

which implies that

$$\mathbf{T} = T_{km} e_k e_m, \ \forall \ \mathbf{T} \in \mathcal{L}.$$

This shows that $\{e_k e_m\}_{k,m=1}^n$ is a basis in the vector space \mathcal{L} with dimension n^2 . By using (2.3), the components of the tensor **T** in this basis can be written as

$$T_{km} = e_k \cdot \mathbf{T} e_m. \tag{2.4}$$

These components can also be represented by $n \times n$ matrix

$$\mathbf{T} = [T_{km}] = \begin{pmatrix} T_{11} & T_{12} & \dots & T_{1n} \\ T_{21} & T_{22} & \dots & T_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ T_{n1} & T_{n2} & \dots & T_{1n} \end{pmatrix}$$

Assume that $\{e_k e_m\}_{k,m=1}^n$ and $\{e'_r e'_s\}_{r,s=1}^n$ are the two bases in \mathcal{L} correspond the two orthonormal bases $\{e_k\}_{k=1}^n$ and $\{e'_k\}_{k=1}^n$ in V_n . We can write the components of the tensor **T** in these bases as

$$\mathbf{T} = T_{km} e_k e_m = T'_{rs} e'_r e'_s.$$
(2.5)

Thus with the help of equations (2.1), (2.4) and (2.5), we have

$$T_{km} = e_k \cdot \mathbf{T} e_m = (Q_{kj} e'_j) \cdot \mathbf{T} (Q_{ml} e'_l)$$
$$= Q_{kj} Q_{ml} T e'_j e'_l$$
$$= Q_{kj} Q_{ml} T'_{jl}.$$

This describes the transformation law of the components of a tensor corresponding the change of basis in \mathcal{L} which can also be written in matrix form as

$$\mathbf{T} = \mathbf{Q}\mathbf{T}'\mathbf{Q}^T.$$

The above result is equivalent to

$$\mathbf{T}' = \mathbf{Q}^T \mathbf{T} \mathbf{Q},$$

which, in component form, becomes

$$T_{rs}' = Q_{kr}Q_{ml}e_{j}'T_{km}$$

2.1.2 Tensor of higher order

A general tensor of rank r in n dimensions, is an entity that contains n^r components denoted as $T_{i_1i_2i_3...i_r}$ $(i_1, i_2, ..., i_r = 1, 2, ..., n)$. Consider a vector space of all tensors of rank r, say, \mathcal{L}_r and assume that $\{e_{i_1}e_{i_2}...e_{i_r}\}_{i_1,i_2,...,i_r=1}^n$ and $\{e'_{s_1}e'_{s_2}...e'_{s_r}\}_{s_1,s_2,...,s_r=1}^n$ are the basis in \mathcal{L}_r . The components of above tensor can be expressed as a linear combination of members of these bases. The transformation law of the components of such a tensor corresponding the change of basis in the vector space \mathcal{L}_r can be written as

$$T_{s_1s_2s_3\ldots s_r}' = Q_{i_1s_1}Q_{i_2s_2}Q_{i_3s_3}\ldots Q_{i_rs_r}T_{i_1i_2i_3\ldots i_r} \quad (s_1,s_2,\ldots,s_r=1,2,\ldots,n).$$

We note that a vector is a tensor of rank one while a scalar is a tensor of rank zero.

2.1.3 Symmetric and antisymmetric tensors

A tensor $T_{i_1i_2i_3...i_r}$ is said to be symmetric with respect to the indices (any two) i_1 and i_3 if

$$T_{i_1 i_2 i_3 \dots i_r} = T_{i_3 i_2 i_1 \dots i_r}$$

and it is said to be antisymmetric with respect to the indices (any two) i_1 and i_3 if

$$T_{i_1 i_2 i_3 \dots i_r} = -T_{i_3 i_2 i_1 \dots i_r}$$

Any tensor can be written as a sum of symmetric and antisymmetric tensors. For instance,

$$T_{ij} = \frac{1}{2}(T_{ij} + T_{ji}) + \frac{1}{2}(T_{ij} - T_{ji}), \ T_{ji}$$
 is the transpose of tensor T_{ij} .

2.1.4 Principal values and principal directions of a symmetric tensor

Let T be a second order symmetric tensor. If u is a unit vector and λ is a scalar such that

$$T\mathbf{u} = \lambda \mathbf{u}$$

or in components form

$$T_{ij}u_i = \lambda u_j,$$

then **u** is called *principal direction* or *principal axis* for the tensor T_{ij} and λ is called its principal value. We can write the above equation as

$$(T_{ij} - \lambda \delta_{ij})u_i = 0,$$

in matrix form

$$\begin{pmatrix} T_{11} - \lambda & T_{12} & T_{13} \\ T_{12} & T_{22} - \lambda & T_{23} \\ T_{13} & T_{23} & T_{33} - \lambda \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

Since u_i is a unit vector (a nonzero vector), the determinant of $T_{ij} - \lambda \delta_{ij}$ must vanish. The three roots of the following characteristic equation

$$\begin{vmatrix} T_{11} - \lambda & T_{12} & T_{13} \\ T_{12} & T_{22} - \lambda & T_{23} \\ T_{13} & T_{23} & T_{33} - \lambda \end{vmatrix} = 0$$

are called *principal values* of the tensor.

It is easily shown that for a symmetric tensor all the principal values are real, then there are three principal directions or principal axes. If principal values are distinct, then three principal directions are mutually orthogonal. If any two of the principal values are equal, then the tensor has the diagonal form and it is independent of the choice of corresponding axis. And if all the principal values are equal, then any direction is a principal direction. A set of mutually orthogonal directions exist for a symmetric tensor of order 2. This defines a Cartesian coordinate system.

2.2 Generalized Hooke's Law

A medium is said to be elastic if it returns to its original state after the external forces are removed. This return to the original state is due to the internal stress. There is a one to one correspondence between stress and strain. Let us denote stress and strain tensors by T_{ij} and S_{ij} , respectively. We assume that T_{ij} is a function of S_{ij} , that is $T_{ij}(S_{ij})$. It is known from experiments that the elastic behaviour of most substances is adequately described (for small deformations) by the first order term in the Taylor expansion of the equation:

$$T_{ij}(S_{kl}) = T_{ij}(0) + \frac{\partial T_{ij}}{\partial S_{kl}}|_{S_{kl}=0}S_{kl} + \frac{\partial^2 T_{ij}}{\partial S_{kl}\partial S_{mn}}|_{\substack{S_{kl}=0\\S_{mn}=0}}S_{kl}S_{mn} + \dots$$

or, since $T_{ij}(0) = 0$, therefore

$$T_{ij} = c_{ijkl} S_{kl}, (2.6)$$

where

$$c_{ijkl} = \frac{\partial T_{ij}}{\partial S_{kl}}|_{S_{kl}=0}.$$
(2.7)

Equation (2.6) is called generalized Hook's Law. This law of proportionality between stress and strain was first stated in the 17th century by Hooke, for the case of a stretched elastic string.

2.2.1 Elasticity tensor

The coefficients c_{ijkl} in the generalized Hook's Law describes the most general linear relationship between the two second rank tensors T_{ij} and S_{kl} , are the components of a fourth rank tensor called the *elastic stiffness tensor* or *elasticity tensor*.

A tensor of rank four, in three dimensions, has $3^4 = 81$ components. Since the tensors T_{ij} and S_{kl} are symmetric, the elastic constants defined by Hooke's Law are unaffected when either the first two or the last two indices are interchanged, so that

$$c_{ijkl} = c_{jikl}$$
 and $c_{ijkl} = c_{ijlk}$.

In terms of displacements, Hooke's law in (2.6) becomes

$$T_{ij} = \frac{1}{2}c_{ijkl}\frac{\partial u_k}{\partial u_l} + \frac{1}{2}c_{ijkl}\frac{\partial u_l}{\partial u_k}$$

and since $c_{ijkl} = c_{ijlk}$ the two summations on the right are equal, so that

$$T_{ij} = c_{ijkl} \frac{\partial u_l}{\partial u_k}.$$

Due to the above symmetry relations the number of independent elastic constants reduces from 81 to 36. Indeed, a pair of unordered indices (i, j) can give only six independent values. These are numbered 1 to 6 according to the following convention

$$(11) \longleftrightarrow 1 \qquad (22) \longleftrightarrow 2 \qquad (33) \longleftrightarrow 3$$
$$(23) = (32) \longleftrightarrow 4 \quad (13) = (31) \longleftrightarrow 5 \quad (12) = (21) \longleftrightarrow 6$$
$$(2.8)$$

The independent elastic moduli can thus be represented in terms of only two indices α and β , with values 1 to 6, corresponding to a 6 × 6 square matrix with 36 entries, such that

$$c_{\alpha\beta} = c_{ijkl},$$

where α is related to (ij) and β to (kl). For example, $c_{14} = c_{1123} = c_{1132}$, $c_{56} = c_{1312} = c_{1321} = c_{1312} = c_{3112}$. This notation was introduced by Voigt [37] and is called the matrix notation to distinguish it from the tensor notation c_{ijkl} , can be extended to the stresses and strains. Thus Hooke's law, given by (2.6), can be written

$$T_{\alpha} = c_{\alpha\beta}S_{\beta} \ (\alpha, \beta = 1, 2, ..., 6.),$$
 (2.9)

where, T_{α} are defined as follows

$$T_1 = T_{11}, T_2 = T_{22}, T_3 = T_{33}, T_4 = T_{23}, T_5 = T_{13}, T_6 = T_{12}.$$

In order to to show that (2.9) gives Hooke's law correctly, we must define S_{β} as

$$S_1 = S_{11}, S_2 = S_{22}, S_3 = S_{33}, S_4 = 2S_{23}, S_5 = 2S_{13}, S_6 = 2S_{12}.$$

For instance, if $\alpha = 2$, we have

$$T_2 = c_{2\beta}S_\beta$$

= $c_{21}S_1 + c_{22}S_2 + c_{23}S_3 + c_{24}S_4 + c_{25}S_5 + c_{26}S_6,$

and

$$T_{22} = c_{22kl}S_{kl}$$

= $c_{2211}S_{11} + c_{2222}S_{22} + c_{2233}S_{33} + 2c_{2223}S_{23} + 2c_{2213}S_{13} + 2c_{2212}S_{12}.$

From this, we can easily identify T_2 and T_{22} .

Elastic energy and symmetry of elasticity tensor

The existence of elastic potential energy defines an elastic continuum [24]. This implies that c_{ijkl} is invariant under permutations of pairs of subscripts ij and kl. This can be derived as follows.

The expression of elastic potential energy is [24]

$$W = \frac{1}{2}c_{ijkl}S_{kl}.$$

Differentiating both sides of these equations with respect to S_{ij} , S_{kl} , respectively, we get

$$\frac{\partial^2 W}{\partial S_{ij} S_{kl}} = c_{ijkl}, \qquad i, j, k, l = \{1, 2, 3\}.$$

If W has continuous first and second order derivatives, then we can write [25]

$$\frac{\partial^2 W}{\partial S_{ij} S_{kl}} = \frac{\partial^2 W}{\partial S_{kl} S_{ij}}$$

which implies that

$$c_{ijkl} = c_{klij}.$$

2.2.2 Compliance tensor

If we write strain in terms of stress, that is to invert Hooke's law as

$$S_{ij} = s_{ijkl} T_{kl}, \tag{2.10}$$

where s_{ijkl} represents the compliance coefficients and form a fourth rank tensor called the *compliance tensor*. This tensor also has the same properties as the elasticity tensor has, so that

$$s_{ijkl} = s_{jikl}$$
 and $s_{ijkl} = s_{ijlk}$.

Similarly, we can write (2.9), in terms of S_{α} as

$$S_{\alpha} = s_{\alpha\beta}T_{\beta},$$

where the matrix $s_{\alpha\beta}$ called compliance matrix is the inverse of the matrix $c_{\alpha\beta}$, that is

$$s_{\alpha\beta}c_{\beta\gamma} = \delta_{\alpha\gamma},$$

where $\delta_{\alpha\gamma}$ is the six-dimensional Kronecker delta. The relation between $s_{\alpha\beta}$ and s_{ijkl} is given by

$$s_{\alpha\beta} = 2^p s_{ijkl},$$

where p is the number of indices greater than 3 in the pair (α, β) . For example,

$$s_{41} = 2s_{2311}, s_{42} = 2s_{2322}, s_{43} = 2s_{2333}, s_{44} = 4s_{2323}, s_{45} = 4s_{2313}, s_{46} = 4s_{2312},$$
etc.

2.3 Mehrabadi and Cowin Formalism

The fourth rank elasticity tensor c_{ijkl} is defined through the generalized Hooke's law

$$T_{ij} = c_{ijkl} S_{kl} \tag{2.11}$$

where T_{ij} and S_{kl} respectively denote the stress tensor and the strain tensor.

In this formalism, Mehrabadi and Cowin [11] have introduced a cartesian basis in three dimensions to construct a cartesian basis in six dimensions. Let us denote the three dimensional cartesian basis vectors by \mathbf{e}_i (i = 1, 2, 3) and those in six dimensions by $\hat{\mathbf{e}}_{\alpha}$ ($\alpha = 1, ..., 6$). These two bases are related by the following equations

$$\hat{\mathbf{e}}_{1} = \mathbf{e}_{1} \otimes \mathbf{e}_{1}, \ \hat{\mathbf{e}}_{4} = \frac{1}{\sqrt{2}} (\mathbf{e}_{2} \otimes \mathbf{e}_{3} + \mathbf{e}_{3} \otimes \mathbf{e}_{2}),$$

$$\hat{\mathbf{e}}_{2} = \mathbf{e}_{2} \otimes \mathbf{e}_{2}, \ \hat{\mathbf{e}}_{5} = \frac{1}{\sqrt{2}} (\mathbf{e}_{1} \otimes \mathbf{e}_{3} + \mathbf{e}_{3} \otimes \mathbf{e}_{1}),$$

$$\hat{\mathbf{e}}_{3} = \mathbf{e}_{3} \otimes \mathbf{e}_{3}, \ \hat{\mathbf{e}}_{6} = \frac{1}{\sqrt{2}} (\mathbf{e}_{1} \otimes \mathbf{e}_{2} + \mathbf{e}_{2} \otimes \mathbf{e}_{1}),$$
(2.12)

where \otimes denotes the tensor product. The six-dimensional base vectors $\hat{\mathbf{e}}_1, ..., \hat{\mathbf{e}}_6$ may have two meanings. That is, they behaves as vectors in six dimensional space (1, 0, 0, 0, 0, 0, 0), ...(0, 0, 0, 0, 0, 1)as well as they can be considered as special second rank tensors in three dimensional space

$$\left(\begin{array}{rrrr}1 & 0 & 0\\0 & 0 & 0\\0 & 0 & 0\end{array}\right), \dots, \frac{1}{\sqrt{2}}\left(\begin{array}{rrrr}0 & 1 & 0\\1 & 0 & 0\\0 & 0 & 0\end{array}\right)$$

We define six dimensional stress and strain vectors,

$$\hat{\mathbf{T}} = \begin{pmatrix} T_{11} \\ T_{22} \\ T_{33} \\ \sqrt{2}T_{23} \\ \sqrt{2}T_{13} \\ \sqrt{2}T_{12} \end{pmatrix}, \hat{\mathbf{S}} = \begin{pmatrix} S_{11} \\ S_{22} \\ S_{33} \\ \sqrt{2}S_{23} \\ \sqrt{2}S_{23} \\ \sqrt{2}S_{13} \\ \sqrt{2}S_{12} \end{pmatrix}$$

The components of stress, strain and elasticity tensor with respect to the three and six dimensional bases are respectively related by the following equations

$$T_{ij}e_i \otimes e_j = T_{\alpha}\hat{e}_{\alpha},$$
$$S_{kl}e_k \otimes e_l = \hat{S}_{\beta}\hat{e}_{\beta},$$
$$c_{ijkl}e_i \otimes e_j \otimes e_k \otimes e_l = \hat{c}_{\alpha\beta}\hat{e}_{\alpha} \otimes \hat{e}_{\beta}$$

^

If we write the relation between three and six dimensional bases in a concise manner, that is if

$$\hat{e}_{\alpha(i,j)} = 2^{-\frac{1}{2-\delta_{ij}}} (\hat{e}_i \otimes \hat{e}_j + \hat{e}_j \otimes \hat{e}_i),$$

where $\alpha(i,j) = i\delta_{ij} + (9-i-j)$. Also define $\hat{T}_{\alpha(i,j)} = 2^{\frac{1}{2-\delta_{ij}}}T_{ij}$ and $\hat{S}_{\beta(i,j)} = 2^{\frac{1}{2-\delta_{ij}}}S_{ij}$, where, i, j = 1, 2, 3 and $\alpha = 1, ..., 6$. Thus in second rank tensor notations, we can write (2.9) as

$$\hat{T}_{\alpha} = \hat{c}_{\alpha\beta}\hat{S}_{\beta}, \,\, \hat{\mathbf{T}} = \hat{\mathbf{c}}\hat{\mathbf{S}},\tag{2.13}$$

where $\hat{\mathbf{T}}$ and $\hat{\mathbf{S}}$ are 1 × 6 column matrices and $\hat{\mathbf{c}}$ is the 6 × 6 matrix. The matrix $\hat{\mathbf{c}}$ has the following representation

$$\mathbf{\hat{c}}_{\alpha\beta} = \begin{pmatrix} c_{11} & c_{12} & c_{13} & \sqrt{2}c_{14} & \sqrt{2}c_{15} & \sqrt{2}c_{16} \\ c_{12} & c_{22} & c_{23} & \sqrt{2}c_{24} & \sqrt{2}c_{25} & \sqrt{2}c_{26} \\ c_{13} & c_{23} & c_{33} & \sqrt{2}c_{34} & \sqrt{2}c_{35} & \sqrt{2}c_{36} \\ \sqrt{2}c_{14} & \sqrt{2}c_{24} & \sqrt{2}c_{34} & 2c_{44} & 2c_{45} & 2c_{46} \\ \sqrt{2}c_{15} & \sqrt{2}c_{25} & \sqrt{2}c_{35} & 2c_{45} & 2c_{55} & 2c_{56} \\ \sqrt{2}c_{16} & \sqrt{2}c_{26} & \sqrt{2}c_{36} & 2c_{46} & 2c_{56} & 2c_{66} \end{pmatrix}$$

Where $c_{\alpha\beta}$ is a symmetric matrix as discussed in section 2.2.1, that is $c_{ijkl} = c_{klij}$. Mehrabadi and Cowin [11] have constructed a six dimensional rotation matrix $\hat{\mathbf{Q}}$ from a given three dimensional rotation matrix \mathbf{Q} as follows.

By the transformation law, the bases e_i and e_i^\prime are related by

$$e'_i = Q_{ij}e_j, \ i, j = 1, 2, 3,$$
(2.14)

where **Q** is an orthogonal tensor in three dimensions. The bases \hat{e}_i and \hat{e}'_i are related by

$$\hat{e}'_{i} = \hat{Q}_{\alpha\beta}\hat{e}_{\beta}, \ \alpha, \beta = 1, ..., 6,$$
 (2.15)

where $\hat{\mathbf{Q}}$ is an orthogonal tensor in six dimensions. From (2.14) and (2.15), it can be written that

$$\hat{e}'_i \otimes \hat{e}'_j = Q_{ik} Q_{jm} e_k e_m \tag{2.16}$$

and

$$\frac{1}{2}(\hat{e}'_{i}\otimes\hat{e}'_{j}+\hat{e}'_{j}\otimes\hat{e}'_{i}) = \frac{1}{2}(Q_{ik}Q_{jm}+Q_{im}Q_{jk})e_{k}\otimes e_{m}.$$
(2.17)

Then from equation (2.15) and (2.12), it follows that

$$\frac{1}{2}(Q_{ik}Q_{jm} + Q_{im}Q_{jk})e_i \otimes e_j \otimes e_k \otimes e_m = \hat{Q}_{\alpha\beta}\hat{e}_{\alpha}\hat{e}_{\beta}.$$
(2.18)

From this formula, the relationship between the components of \mathbf{Q} and $\hat{\mathbf{Q}}$ can be constructed in the form of the following matrix

$$\hat{\mathbf{Q}} = \begin{pmatrix} \hat{Q}_{11} & \hat{Q}_{12} & \hat{Q}_{13} & \hat{Q}_{14} & \hat{Q}_{15} & \hat{Q}_{16} \\ \hat{Q}_{21} & \hat{Q}_{22} & \hat{Q}_{23} & \hat{Q}_{24} & \hat{Q}_{25} & \hat{Q}_{26} \\ \hat{Q}_{31} & \hat{Q}_{32} & \hat{Q}_{33} & \hat{Q}_{34} & \hat{Q}_{35} & \hat{Q}_{36} \\ \hat{Q}_{41} & \hat{Q}_{42} & \hat{Q}_{43} & \hat{Q}_{44} & \hat{Q}_{45} & \hat{Q}_{46} \\ \hat{Q}_{51} & \hat{Q}_{52} & \hat{Q}_{53} & \hat{Q}_{54} & \hat{Q}_{55} & \hat{Q}_{56} \\ \hat{Q}_{61} & \hat{Q}_{62} & \hat{Q}_{63} & \hat{Q}_{64} & \hat{Q}_{65} & \hat{Q}_{66} \end{pmatrix},$$

$$(2.19)$$

where

$$\begin{split} \hat{Q}_{11} &= Q_{11}^2, \hat{Q}_{12} = Q_{12}^2, \hat{Q}_{21} = Q_{21}^2, \hat{Q}_{13} = Q_{13}^2, \hat{Q}_{31} = Q_{31}^2 \\ \hat{Q}_{14} &= \sqrt{2}Q_{12}Q_{13}, \hat{Q}_{41} = \sqrt{2}Q_{21}Q_{31}, \\ \hat{Q}_{15} &= \sqrt{2}Q_{11}Q_{13}, \hat{Q}_{51} = \sqrt{2}Q_{11}Q_{31}, \\ \hat{Q}_{16} &= \sqrt{2}Q_{11}Q_{12}, \hat{Q}_{61} = \sqrt{2}Q_{11}Q_{21}, \\ \hat{Q}_{22} &= Q_{22}^2, \hat{Q}_{23} = Q_{23}^2, \hat{Q}_{32} = Q_{32}^2, \\ \hat{Q}_{24} &= \sqrt{2}Q_{22}Q_{23}, \hat{Q}_{42} = \sqrt{2}Q_{22}Q_{32}, \\ \hat{Q}_{25} &= \sqrt{2}Q_{21}Q_{23}, \hat{Q}_{52} = \sqrt{2}Q_{12}Q_{22}, \\ \hat{Q}_{26} &= \sqrt{2}Q_{22}Q_{21}, \hat{Q}_{62} = \sqrt{2}Q_{12}Q_{22}, \\ \hat{Q}_{33} &= Q_{33}^2, \hat{Q}_{34} = \sqrt{2}Q_{33}Q_{32}, \hat{Q}_{43} = \sqrt{2}Q_{23}Q_{33}, \\ \hat{Q}_{35} &= \sqrt{2}Q_{33}Q_{31}, \hat{Q}_{53} = \sqrt{2}Q_{13}Q_{33}, \\ \hat{Q}_{36} &= \sqrt{2}Q_{31}Q_{32}, \hat{Q}_{63} = \sqrt{2}Q_{13}Q_{23}, \\ \hat{Q}_{44} &= Q_{22}Q_{33} + Q_{23}Q_{32}, \\ \hat{Q}_{45} &= Q_{21}Q_{33} + Q_{31}Q_{23}, \hat{Q}_{54} = Q_{21}Q_{33} + Q_{31}Q_{23}, \\ \hat{Q}_{46} &= Q_{21}Q_{32} + Q_{31}Q_{22}, \hat{Q}_{64} = Q_{12}Q_{23} + Q_{22}Q_{13}, \\ \hat{Q}_{55} &= Q_{11}Q_{33} + Q_{13}Q_{31}, \\ \hat{Q}_{56} &= Q_{11}Q_{32} + Q_{31}Q_{12}, \hat{Q}_{65} = Q_{11}Q_{23} + Q_{21}Q_{13}, \\ \hat{Q}_{66} &= Q_{11}Q_{22} + Q_{21}Q_{12}. \end{split}$$

With $\hat{\mathbf{Q}}$ defined by above, equation (2.14) becomes a tensor equation in six dimension. It can be shown that orthogonality of \mathbf{Q} implies the orthogonality of $\hat{\mathbf{Q}}$, that is,

$$\mathbf{Q}\mathbf{Q}^T = \mathbf{Q}^T\mathbf{Q} = \mathbf{I} \tag{2.20}$$

implies that

$$\hat{\mathbf{Q}}\hat{\mathbf{Q}}^T = \hat{\mathbf{Q}}^T\hat{\mathbf{Q}} = I \tag{2.21}$$

in order to prove (2.21), consider

$$\mathbf{Q} = \begin{pmatrix} Q_{11} & Q_{12} & Q_{13} \\ Q_{21} & Q_{22} & Q_{23} \\ Q_{31} & Q_{32} & Q_{33} \end{pmatrix}, \ \mathbf{Q}^T = \begin{pmatrix} Q_{11} & Q_{21} & Q_{31} \\ Q_{12} & Q_{22} & Q_{32} \\ Q_{13} & Q_{23} & Q_{33} \end{pmatrix},$$

which gives

$$\mathbf{Q}\mathbf{Q}^{T} = \begin{pmatrix} Q_{11}^{2} + Q_{12}^{2} + Q_{13}^{2} & Q_{11}Q_{21} + Q_{12}Q_{22} + Q_{13}Q_{23} & Q_{11}Q_{31} + Q_{12}Q_{32} + Q_{13}Q_{33} \\ Q_{11}Q_{21} + Q_{12}Q_{22} + Q_{13}Q_{23} & Q_{21}^{2} + Q_{22}^{2} + Q_{23}^{2} & Q_{21}Q_{31} + Q_{22}Q_{32} + Q_{23}Q_{33} \\ Q_{11}Q_{31} + Q_{12}Q_{32} + Q_{13}Q_{33} & Q_{21}Q_{31} + Q_{22}Q_{32} + Q_{23}Q_{33} & Q_{31}^{2} + Q_{32}^{2} + Q_{33}^{2} \\ & (2.22) \end{pmatrix}$$

Using (2.22) in (2.20), we have the following relations

$$Q_{11}^2 + Q_{12}^2 + Q_{13}^2 = 1, (2.23a)$$

$$Q_{21}^2 + Q_{22}^2 + Q_{23}^2 = 1, (2.23b)$$

$$Q_{31}^2 + Q_{32}^2 + Q_{33}^2 = 1, (2.23c)$$

$$Q_{11}Q_{21} + Q_{12}Q_{22} + Q_{13}Q_{23} = 0, (2.23d)$$

$$Q_{11}Q_{31} + Q_{12}Q_{32} + Q_{13}Q_{33} = 0, (2.23e)$$

$$Q_{21}Q_{31} + Q_{22}Q_{32} + Q_{23}Q_{33} = 0. (2.23f)$$

For orthogonality of $\hat{\mathbf{Q}}$, we need to check each element of the product matrix $\hat{\mathbf{Q}}\hat{\mathbf{Q}}^{T}$. Let us denote these elements by $\left[\hat{\mathbf{Q}}\hat{\mathbf{Q}}^{T}\right]_{ij}$, i, j = 1, 2, ..., 6. We can compute these components as follows

$$\begin{split} \left[\hat{\mathbf{Q}} \hat{\mathbf{Q}}^T \right]_{11} &= Q_{11}^4 + Q_{12}^4 + Q_{13}^4 + 2Q_{11}^2 Q_{12}^2 + 2Q_{11}^2 Q_{13}^2 + 2Q_{12}^2 Q_{13}^2 \\ &= (Q_{11}^2 + Q_{12}^2 + Q_{13}^2)^2 \\ &= 1, \text{ using } (2.23a). \end{split}$$

Similarly

$$\begin{split} \left[\hat{\mathbf{Q}} \hat{\mathbf{Q}}^T \right]_{22} &= (Q_{21}^2 + Q_{22}^2 + Q_{23}^2)^2 = 1, \\ \left[\hat{\mathbf{Q}} \hat{\mathbf{Q}}^T \right]_{33} &= (Q_{31}^2 + Q_{32}^2 + Q_{33}^2)^2 = 1, \\ \left[\hat{\mathbf{Q}} \hat{\mathbf{Q}}^T \right]_{12} &= \left[\hat{\mathbf{Q}} \hat{\mathbf{Q}}^T \right]_{21} = (Q_{11}Q_{21} + Q_{12}Q_{22} + Q_{13}Q_{23})^2 = 0, \\ \left[\hat{\mathbf{Q}} \hat{\mathbf{Q}}^T \right]_{13} &= \left[\hat{\mathbf{Q}} \hat{\mathbf{Q}}^T \right]_{31} = (Q_{11}Q_{31} + Q_{12}Q_{32} + Q_{13}Q_{33})^2 = 0, \\ \left[\hat{\mathbf{Q}} \hat{\mathbf{Q}}^T \right]_{23} &= \left[\hat{\mathbf{Q}} \hat{\mathbf{Q}}^T \right]_{32} = (Q_{21}Q_{31} + Q_{22}Q_{32} + Q_{23}Q_{33})^2 = 0, \text{ and so only} \end{split}$$

Thus we have $\hat{\mathbf{Q}}\hat{\mathbf{Q}}^T = \mathbf{I}$, similarly we can show that $\hat{\mathbf{Q}}^T\hat{\mathbf{Q}} = \mathbf{I}$. This proves equation (2.21).

In a special case when **Q** is rotation about x_1 -axis through an angle θ , that is,

$$\mathbf{Q} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & \sin\theta \\ 0 & -\sin\theta & \cos\theta \end{pmatrix},$$

the corresponding matrix $\hat{\mathbf{Q}}$ becomes

1

$$\hat{\mathbf{Q}} = \hat{\mathbf{Q}}(\theta) = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & \cos^2 \theta & \sin^2 \theta & \sqrt{2} \sin \theta \cos \theta & 0 & 0 \\ 0 & \sin^2 \theta & \cos^2 \theta & -\sqrt{2} \sin \theta \cos \theta & 0 & 0 \\ 0 & -\sqrt{2} \sin \theta \cos \theta & \sqrt{2} \sin \theta \cos \theta & \cos^2 \theta - \sin^2 \theta & 0 & 0 \\ 0 & 0 & 0 & 0 & \cos \theta & -\sin \theta \\ 0 & 0 & 0 & 0 & \sin \theta & \cos \theta \end{pmatrix}$$
(2.24)

$\mathbf{2.4}$ **Commuting Operators**

We state a result in the following theorem about commuting operators which is well known if the two operators (matrices) are Hermitian. In quantum mechanics, this result has great significance. If the two operators representing observables commute, the associated observables can be measured at the same time [38]. Two operators \mathbf{A} and \mathbf{B} are said to commute if AB = BA or [A, B] = AB - BA = 0.

Theorem 2.1. If the operators **A** and **B** commute and if one of the operators has an eigenvalue of finite geometric multiplicity, both operators have a common eigenvector; that is, there exists a vector \mathbf{v} such that

$$\mathbf{A}\mathbf{v} = \lambda\mathbf{v}, \ \mathbf{B}\mathbf{v} = \mu\mathbf{v},$$

where λ and μ are scalars.

Proof. Since $\mathbf{A}\mathbf{y} = \lambda \mathbf{y}$ implies that $(\mathbf{A} - \lambda \mathbf{I})\mathbf{y} = 0$, the eigenvectors of \mathbf{A} corresponding to a given eigenvalue λ are elements of the null space for the operator $\mathbf{A} - \lambda \mathbf{I}$. Now if

$$\mathbf{AB} = \mathbf{BA} \Rightarrow (\mathbf{A} - \lambda \mathbf{I})\mathbf{B} = \mathbf{B}(\mathbf{A} - \lambda \mathbf{I}).$$

Since, the null space of one of the commuting operators is an invariant subspace for the other; consequently, the null space of $\mathbf{A} - \lambda \mathbf{I}$ is invariant subspace for **B**. It is known that if a finite dimensional subspace is invariant under an operator, the effect of that operator may be represented by a matrix [26]. Since by hypothesis, the null space of $\mathbf{A} - \lambda \mathbf{I}$ is finite dimensional, therefore \mathbf{B} can be represented by a matrix in this space. If a finite dimensional subspace is invariant under an operator, then there exists an eigenvector of that operator in the corresponding subspace. It follows that \mathbf{B} has an eigenvector \mathbf{v} in the null space of $\mathbf{L} - \lambda \mathbf{I}$; consequently, we have

$$\mathbf{B}\mathbf{v} = \mu\mathbf{v}, \ (\mathbf{A} - \lambda\mathbf{I})\mathbf{v} = 0 \Rightarrow \mathbf{A}\mathbf{v} = \lambda\mathbf{v},$$

which proves the theorem.

As an application of theorem 2.1, we consider the classical orbital angular momentum

$$\mathbf{L}=\mathbf{r}\times\mathbf{P},$$

where $\mathbf{r} = (x, y, z)$ is the position vector and $\mathbf{P} = (p_x, p_y, p_z)$ is the (linear) momentum vector for a particle [39]. The components of \mathbf{L} are

$$L_x = yp_z - zp_y$$
$$L_y = zp_x - xp_z$$
$$L_z = xp_y - yp_x$$

and the square magnitude of the total angular momentum vector \mathbf{L} is

$$L^2 = L_x^2 + L_y^2 + L_z^2.$$

The quantum mechanical operators corresponding to these observables are given by

$$\begin{split} \hat{L}_x &= -i\hbar (y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y})\\ \hat{L}_y &= -i\hbar (z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z})\\ \hat{L}_z &= -i\hbar (x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x})\\ \hat{L}^2 &= \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2. \end{split}$$

We can show that

$$\begin{aligned} [\hat{L}_x, \hat{L}_y] &= i\hbar \hat{L}_z \\ [\hat{L}_y, \hat{L}_z] &= i\hbar \hat{L}_x \\ [\hat{L}_z, \hat{L}_x] &= i\hbar \hat{L}_y. \end{aligned}$$
(2.25)

and

$$[\hat{L}^2, \hat{L}_x] = [\hat{L}^2, \hat{L}_y] = [\hat{L}^2, \hat{L}_z] = 0.$$
(2.26)

It is clear from (2.25) that the individual components of \hat{L} don't have common eigenstates with one another (except for a special case of zero angular momentum). But (2.26) shows that the components of \hat{L} have simultaneous eigenfunctions with \hat{L}^2 . For example, we can say that \hat{L}^2 and \hat{L}_z have simultaneous eigenfunctions. That is, there are states that are eigenfunctions of both \hat{L}^2 and \hat{L}_z . Let us call these eigenfunctions φ_{lm} such that

$$\hat{L}^2 \varphi_{lm} = \hbar^2 l(l+1)\varphi_{lm}, \ (l=0,1,2,\ldots)$$
$$\hat{L}_z \varphi_{lm} = \hbar m \varphi_{lm} (m=-l,\ldots,+l).$$

2.5 Material Symmetry

The set of all those transformations which preserve the distances between all pairs of points of the body and bring the body into coincidence with itself, describe the symmetry of the body. Such a transformation is said to be a *symmetry transformation*. This set forms a group, which is called the symmetry group of the body. There are three fundamental transformations; *rotation*, *reflection* and *translation*. The set of distance preserving symmetry transformations can be built up from these fundamental transformations. Rotation through an angle about some axis and a mirror reflection in a plane are possible for a body of finite extension, a molecule or a macroscopic form of a mineral. Translation (parallel displacement), can occur only when the body is infinite in extent, for example, an infinite crystal lattice.

Let us write the elastic stiffnesses c_{ijkl} , as the components of fourth rank elasticity tensor. Under an orthogonal transformation

$$x_i^* = Q_{ij} x_j \text{ or } \mathbf{x}^* = \mathbf{Q} \mathbf{x} \tag{2.27}$$

where **Q** is an orthogonal transformation (section 2.1). The elastic stiffnesses c_{ijkl}^* and elastic compliances s_{ijkl}^* referred to x_i^* coordinate system are, respectively,

$$c_{ijkl}^* = Q_{ip}Q_{jq}Q_{kr}Q_{ls}c_{pqrs} \tag{2.28}$$

and

$$s_{ijkl}^* = Q_{ip}Q_{jq}Q_{kr}Q_{ls}s_{pqrs}.$$
(2.29)

When $c_{ijkl}^* = c_{ijkl}$ and $s_{ijkl}^* = s_{ijkl}$, that is

$$c_{ijkl} = Q_{ip}Q_{jq}Q_{kr}Q_{ls}c_{pqrs} \tag{2.30}$$

and

$$s_{ijkl} = Q_{ip}Q_{jq}Q_{kr}Q_{ls}s_{pqrs}, (2.31)$$

the material is said to possess a symmetry with respect to \mathbf{Q} . If (2.30) and (2.31) are satisfied for

$$\mathbf{Q} = \begin{pmatrix} -1 & 0 & 0\\ 0 & -1 & 0\\ 0 & 0 & -1 \end{pmatrix},$$
(2.32)

we say that the anisotropic material possess the symmetry of central inversion. Equations (2.30) and (2.31) are obviously satisfied for \mathbf{Q} given in (2.32) for any c_{ijkl} and s_{ijkl} , respectively. Hence all anisotropic elastic materials have the symmetry of central inversion.

The transformation (2.27) represents a rigid body rotation if \mathbf{Q} is a proper orthogonal matrix, i.e., if det $\mathbf{Q} = +1$. When (2.30) and (2.31) are satisfied for a proper orthogonal matrix \mathbf{Q} , the material possesses a *rotational symmetry*. For example,

$$\mathbf{Q}(\theta) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & \sin\theta \\ 0 & -\sin\theta & \cos\theta \end{pmatrix}$$
(2.33)

represents a rotation about x_1 -axis through an angle θ . An orthogonal transformation **Q** is called a *mirror reflection* in a plane if

$$\mathbf{Q} = \mathbf{I} - 2\mathbf{n}\mathbf{n}^T \tag{2.34}$$

in which **n** is a unit vector normal to the plane of reflection. The matrix form of (2.28) is

$$\mathbf{Q} = \begin{pmatrix} 1 - 2n_1^2 & -2n_1n_2 & -2n_1n_3 \\ -2n_1n_2 & 1 - 2n_2^2 & -2n_2n_3 \\ -2n_1n_3 & -2n_2n_3 & 1 - 2n_3^2 \end{pmatrix}$$

If **m** is any vector on the plane, i.e., $\mathbf{m} \perp \mathbf{n}$,

$$\mathbf{Qn} = -\mathbf{n}, \, \mathbf{Qm} = \mathbf{m}. \tag{2.35}$$

Thus a vector normal to the plane of reflection reverses its direction due to transformation but a vector on the plane of reflection is unaltered. When (2.30) and (2.31) are satisfied for the matrix \mathbf{Q} of (2.34), the material possesses a *plane of symmetry*. For example, let

$$\mathbf{n}^T = [0, \cos\theta, \sin\theta].$$

The plane of symmetry contains the x_1 -axis. The matrix **Q** of (2.34) has the following expression

$$\mathbf{Q}(\theta) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -\cos 2\theta & -\sin 2\theta \\ 0 & -\sin 2\theta & \cos 2\theta \end{pmatrix}, \quad -\frac{\pi}{2} < \theta \le \frac{\pi}{2}.$$
 (2.36)

The matrix in (2.36) is an improper orthogonal matrix because det $\mathbf{Q} = -1$. Since θ and $\theta + \pi$ represents the same plane, where, $-\frac{\pi}{2} < \theta \leq \frac{\pi}{2}$. At $\theta = 0$,

$$\mathbf{Q}(0) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$
 (2.37)

This represents a reflection about the plane $x_3 = 0$. When (2.30) and (2.31) are satisfied for the matrix $\mathbf{Q}(0)$ of (2.35), the material has a plane of symmetry at $x_3 = 0$. If (2.30) and (2.31) are satisfied for the matrix $\mathbf{Q}(\theta)$ of (2.36), the material is *transversely isotropic*. The x_1 -axis is the axis of symmetry.

2.5.1 Effect of material symmetry on elastic constants

The elastic stiffness matrix \mathbf{c} and compliance matrix \mathbf{s} are 6×6 matrices contain 21 independent elastic constants. The number of independent constants is reduced when the material possesses a certain material symmetry. We will discuss reduction in the number of these components of the tensors describing isotropic and anisotropic materials as follows.

Isotropic materials

A material is said to be *isotropic* if its properties are same in all directions (e.g. many structural metals such as *steel* and *aluminium*). This will happen if the tensor c_{ijkl} is an isotropic tensor (i.e. a tensor whose components remains invariant in all choices of reference frames). An isotropic material possesses infinitely many rotational symmetries and planes of reflection symmetry. A scalar and the Identity tensor δ_{ij} are the quantities which are unaffected by the coordinate transformations. As δ_{ij} is symmetric, i.e. $\delta_{ij} = \delta_{ji}$, therefore the only distinct combinations containing the four indices i, j, k, l are $\delta_{ij}\delta_{kl}, \delta_{ik}\delta_{jl}$ and $\delta_{il}\delta_{jk}$. Therefore c_{ijkl} can be written as:

$$c_{ijkl} = \lambda \delta_{ij} \delta_{kl} + \mu (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) \tag{2.38}$$

where λ and μ are Lamé constants. The tensor c_{ijkl} given in (2.27) satisfies (2.30) for any orthogonal matrix **Q**. From this we have

$$c_{\alpha\beta} = \begin{pmatrix} \lambda + 2\mu & \lambda & \lambda & 0 & 0 & 0 \\ \lambda & \lambda + 2\mu & \lambda & 0 & 0 & 0 \\ \lambda & \lambda & \lambda + 2\mu & 0 & 0 & 0 \\ 0 & 0 & 0 & \mu & 0 & 0 \\ 0 & 0 & 0 & 0 & \mu & 0 \\ 0 & 0 & 0 & 0 & 0 & \mu \end{pmatrix}$$
(2.39)

Thus instead of 21, it has only 2 independent components.

Triclinic materials

These are the most general anisotropic materials having no planes of symmetry. They have only a center of symmetry which impose no condition, so all these materials have 21 independent constants and this number will not be reduced further. These constants can be arranged in the following matrix form

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

$$(2.40)$$

Monoclinic materials

Monoclinic materials possesses a plane of symmetry. Taking the dyad axis or axis of symmetry along x_3 -axis. The symmetry plane will be at $x_1 = 0$. The transformation of coordinates is given by $x'_1 = -x_1$, $x'_2 = -x_2$, $x'_3 = x_3$. Therefore the transformation matrix will be

$$\mathbf{Q} = \begin{pmatrix} -1 & 0 & 0\\ 0 & -1 & 0\\ 0 & 0 & 1 \end{pmatrix}.$$
 (2.41)

By using (2.41) into (2.30), the elastic constants in which the index 1 occurs once or three times become zero. We have the following matrix form

$$c_{\alpha\beta} = \begin{pmatrix} c_{11} & c_{12} & c_{13} & 0 & 0 & c_{16} \\ c_{12} & c_{22} & c_{23} & 0 & 0 & c_{26} \\ c_{13} & c_{23} & c_{33} & 0 & 0 & c_{36} \\ 0 & 0 & 0 & c_{44} & c_{45} & 0 \\ 0 & 0 & 0 & c_{45} & c_{55} & 0 \\ c_{16} & c_{26} & c_{36} & 0 & 0 & c_{66} \end{pmatrix}.$$
 (2.42)

Orthotropic materials

There are three symmetry planes for these materials. Taking three dyad axes along the coordinate axis and apply the same argument to each coordinate axis as above, where the

only non zero components are those having indices 2 or 4 times. The matrix is

$$c_{\alpha\beta} = \begin{pmatrix} c_{11} & c_{12} & c_{13} & 0 & 0 & 0\\ c_{12} & c_{22} & c_{23} & 0 & 0 & 0\\ c_{13} & c_{23} & c_{33} & 0 & 0 & 0\\ 0 & 0 & 0 & c_{44} & 0 & 0\\ 0 & 0 & 0 & 0 & c_{55} & 0\\ 0 & 0 & 0 & 0 & 0 & c_{66} \end{pmatrix}.$$
(2.43)

Cubic materials

Cubic materials have at least four triad axes and three dyad axes. Taking the dyad axes along the coordinate axes. A rotation by $\frac{2\pi}{3}$ about the triad axis directed along the diagonal gives a cyclic permutation of the axes. The elastic constants c_{ijkl} are unchanged for the cyclic permutation of the indices $123 \rightarrow 231 \rightarrow 312$. This implies that

$$c_{1111} = c_{2222}, \ c_{2222} = c_{3333}, \ \text{etc.}$$

The matrix (2.43) for cubic materials becomes

$$c_{\alpha\beta} = \begin{pmatrix} c_{11} & c_{12} & c_{12} & 0 & 0 & 0\\ c_{12} & c_{11} & c_{12} & 0 & 0 & 0\\ c_{12} & c_{12} & c_{11} & 0 & 0 & 0\\ 0 & 0 & 0 & c_{44} & 0 & 0\\ 0 & 0 & 0 & 0 & c_{44} & 0\\ 0 & 0 & 0 & 0 & 0 & c_{44} \end{pmatrix}.$$

$$(2.44)$$

Materials with principal axis of order greater than two

If a material remains unchanged after rotating through an angle $\frac{2\pi}{n}$, the material has principal axis A_n , an *n*-fold axis of rotation. For materials of *trigonal, tetragonal and hexagonal* systems, the value of *n* is greater than 2. That is n = 3, 4 and 6 respectively. The rotation matrix **Q** about this principal axis is not diagonal now. For instance, taking A_n along x_3 -axis, we have

$$\mathbf{Q} = \begin{pmatrix} \cos\theta & \sin\theta & 0\\ -\sin\theta & \cos\theta & 0\\ 0 & 0 & 1 \end{pmatrix}, \text{ where } \theta = \frac{2\pi}{n} \neq \pi,$$
(2.45)

which is not a diagonal matrix. In this case, the invariance condition (2.30) becomes more complex. Therefore we diagonalize the matrix in (2.45) and get the orthonormal basis $\xi^{(1)} = (\frac{1}{\sqrt{2}}, \frac{i}{\sqrt{2}}, 0)^T$, $\xi^{(2)} = (\frac{i}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0)^T$ and $\xi^{(2)} = (0, 0, 1)^T$. The resulting diagonal matrix is

$$\mathbf{Q} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} & 0\\ \frac{i}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0\\ 0 & 0 & 1 \end{pmatrix}.$$
 (2.46)

let us denote the elastic constants by γ_{ijkl} in this orthonormal basis. The relation (2.30) becomes

$$\gamma_{ijkl} = \lambda^{(i)} \lambda^{(j)} \lambda^{(k)} \lambda^{(l)} \gamma_{ijkl} \tag{2.47}$$

By converting back to the constants c_{ijkl} , we can write

$$c_{ijkl} = Q_{ip}Q_{jq}Q_{kr}Q_{ls}\gamma_{pqrs} \tag{2.48}$$

Use of relation (2.37) leads us to the following matrix form for the **trigonal materials** [40]

$$c_{\alpha\beta} = \begin{pmatrix} c_{11} & c_{12} & c_{13} & c_{14} & -c_{25} & 0\\ c_{12} & c_{11} & c_{13} & -c_{14} & c_{25} & 0\\ c_{13} & c_{13} & c_{33} & c_{34} & c_{35} & 0\\ c_{14} & -c_{14} & 0 & c_{44} & c_{45} & c_{25}\\ -c_{25} & c_{25} & 0 & c_{45} & c_{44} & c_{14}\\ 0 & 0 & 0 & c_{25} & c_{14} & \frac{c_{11}-c_{12}}{2} \end{pmatrix}.$$

$$(2.49)$$

Similarly, for tetragonal materials, we have

1

$$c_{\alpha\beta} = \begin{pmatrix} c_{11} & c_{12} & c_{13} & 0 & 0 & c_{16} \\ c_{12} & c_{11} & c_{13} & 0 & 0 & -c_{16} \\ c_{13} & c_{13} & c_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{44} & 0 \\ c_{16} & -c_{16} & 0 & 0 & 0 & c_{66} \end{pmatrix}$$
(2.50)
and for hexagonal materials, the matrix form becomes

$$c_{\alpha\beta} = \begin{pmatrix} c_{11} & c_{12} & c_{13} & 0 & 0 & 0\\ c_{12} & c_{11} & c_{13} & 0 & 0 & 0\\ c_{13} & c_{13} & c_{33} & 0 & 0 & 0\\ 0 & 0 & 0 & c_{44} & 0 & 0\\ 0 & 0 & 0 & 0 & c_{44} & 0\\ 0 & 0 & 0 & 0 & 0 & \frac{c_{11} - c_{12}}{2} \end{pmatrix}.$$
 (2.51)

2.6 Cowin-Mehrabadi Theorem

At a point in an elastic material, a plane with respect to which the material has reflective symmetry is said to be a plane of symmetry. This section is devoted to the identification of material symmetry for an anisotropic elastic material. That is, given form of c_{ijkl} for an elastic material relative to an arbitrary coordinate system, which of the traditional elastic symmetries it belongs. To solve this problem, we need to find the orientation of the traditional symmetry elements. Mehrabadi and Cowin [28] have proved a Theorem which determines the orientations of the plane of symmetry of a given c_{ijkl} relative to arbitrary coordinate system.

Theorem 2.2. A set of necessary and sufficient conditions for a unit vector \mathbf{n} to be a normal to a plane of symmetry is that it should be a common eigenvector of the following tensors

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

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

$$W_{ik}(\mathbf{n}) = c_{ijkl}m_jm_l,$$

$$W_{ik}(\mathbf{m}) = c_{ijkl}m_jm_l;$$

where \mathbf{m} is any vector perpendicular to \mathbf{n} .

Proof. For necessity of these conditions we have to show that \mathbf{n} is a common eigenvector

of above four tensors satisfying the following equations

$$c_{ijkk}n_j = (c_{pqrr}n_pn_q)n_i; (2.52)$$

$$c_{ilkl}n_k = (c_{pqrq}n_pn_r)n_i \tag{2.53}$$

$$c_{ijkl}n_jn_ln_k = (c_{pqrs}n_pn_qn_rn_s)n_i \tag{2.54}$$

$$c_{ijkl}m_jm_ln_k = (c_{pqrs}n_pm_qn_rm_s)n_i.$$

$$(2.55)$$

To prove (2.52) we multiply both sides of (2.30) by n_i

$$c_{ijkl}n_j = Q_{ip}Q_{jq}Q_{kr}Q_{ls}c_{pqrs}n_j$$
$$= Q_{ip}(Q_{jq}n_j)Q_{kr}Q_{ls}c_{pqrs}$$

Using (2.35)

$$c_{ijkl}n_j = -Q_{ip}Q_{kr}Q_{ls}c_{pqrs}n_q,$$

when l = k,

$$c_{ijkk}n_j = -Q_{ip}Q_{kr}Q_{ks}c_{pqrs}n_q,$$

Since Q is orthogonal, so we have

$$Q_{kr}Q_{ks} = \delta_{rs}$$

and

$$c_{ijkk}n_j = -Q_{ip}\delta_{rs}c_{pqrs}n_q$$
$$= -Q_{ip}c_{pqrr}n_q$$
$$= -(\delta_{ip} - 2n_in_p)c_{pqrr}n_q$$
$$= -c_{iqrr}n_q + 2c_{pqrr}n_in_pn_q.$$

As q and r re dummy indices, so we can write

$$c_{ijkk}n_j = -c_{iqrr}n_q + 2c_{pqrr}n_in_pn_q$$

This implies that

$$c_{ijkk}n_j = (c_{pqrr}n_pn_q)n_i$$

Which proves (2.52). Similarly (2.53)-(2.55) can be proved by applying the same procedure as above [28]. In chapter 4, we shall present a simpler argument to prove the above result.

To prove sufficiency of the conditions, let $x_1 = 0$ is a plane of symmetry so that

$$n_i = \delta_{i1},\tag{2.56}$$

$$m_i = \delta_{i2} \cos \theta + \delta_{i3} \sin \theta, \qquad (2.57)$$

where, θ is an arbitrary constant. As the equations (2.52)-(2.55) are satisfied, using (2.56) into (2.52)-(2.54), we have

$$c_{ijkk}\delta_{i1} = (c_{pqrr}\delta_{p1}\delta_{q1})\delta_{i1},$$

this implies that

$$c_{i1kk} = c_{11rr}\delta_{i1}.$$

For i = 1, equations (2.52)-(2.55) are trivially satisfied. For i = 2, 3, we have

$$c_{21kk} = 0 = c_{31kk}$$

or

$$c_{2111} + c_{2122} + c_{2133} = 0 = c_{3111} + c_{3122} + c_{3133}$$

or

$$c_{16} + c_{26} + c_{36} = 0 = c_{15} + c_{25} + c_{35}$$

$$(2.58)$$

and

$$c_{ilkl}\delta_{i1} = c_{pqrq}\delta_{p1}\delta_{r1}\delta_{i1}$$

this implies that

$$c_{il1l}\delta_{i1} = c_{1q1q}\delta_{i1}.$$

For i = 2, 3, we have

$$c_{2l1l} = 0 = c_{3l1l}$$

or

$$c_{2111} + c_{2212} + c_{213} = 0 = c_{3111} + c_{3212} + c_{3313}$$

or

$$c_{16} + c_{26} + c_{45} = 0 = c_{15} + c_{46} + c_{35}.$$

$$(2.59)$$

Also we have

$$c_{ijkl}\delta_{j1}\delta_{l1}\delta_{k1} = c_{pqrq}\delta_{p1}\delta_{r1}\delta_{s1}\delta_{i1}$$

this implies that

$$c_{i111} = c_{1111}\delta_{i1}.$$

For i = 2, 3, we have

$$c_{2111} = 0 = c_{3111}$$

or

$$c_{16} = 0 = c_{15}.\tag{2.60}$$

Now substitute (2.57) into (2.55), we have

 $c_{ijkl}(\delta_{i2}\cos\theta + \delta_{i3}\sin\theta)(\delta_{j2}\cos\theta + \delta_{j3}\sin\theta)\delta_{k1} = c_{pqrs}\delta_{p1}(\delta_{q2}\cos\theta + \delta_{q3}\sin\theta)\delta_{r1}(\delta_{s2}\cos\theta + \delta_{s3}\sin\theta)\delta_{i1}$ this implies that

$$c_{i212}\cos^2\theta + c_{i213}\cos\theta\sin\theta + c_{i312}\cos\theta\sin\theta + c_{i312}\sin\theta\cos\theta + c_{i313}\sin^2\theta$$
$$= (c_{1212}\cos^2\theta + c_{1213}\cos\theta\sin\theta + c_{1312}\cos\theta\sin\theta + c_{1312}\sin\theta\cos\theta + c_{1313}\sin^2\theta)\delta_{i1}.$$

For $\theta = 0, \frac{\pi}{2}$ and for arbitrary value, respectively, we have

$$c_{i212} = c_{1212}\delta_{i1}$$

$$c_{i313} = c_{1313}\delta_{i1}$$

$$+ c_{i312})\cos\theta\sin\theta = (c_{1213} + c_{i312})\cos\theta\sin\theta\delta_{i1}.$$

For $\theta \neq 0, \frac{\pi}{2}$ the above equation becomes

 (c_{i213})

$$c_{i212} + c_{i312} = c_{1213} + c_{i312}.$$

For i = 1, the above equations are satisfied. For i = 2, 3, we have

$$c_{2212} = 0 = c_{3212}$$

or

$$c_{26} = 0 = c_{46}$$

and

$$c_{2213} + c_{2312} = 0 = c_{3213} + c_{3312}$$

or

$$c_{25} + c_{46} = 0 = c_{45} + c_{36}. (2.61)$$

From (2.58)-(2.61), we have

$$c_{26} = c_{46} = c_{45} = c_{35} = c_{25} = c_{36=0}.$$
(2.62)

As the equations (2.56)-(2.60) are the special cases of (2.52)-(2.55) if unit normal vector **n** is along x_1 -axis, hence **n** is normal to the plane of symmetry. If $x_1 = 0$ is a plane of symmetry, we have

$$c_{15} = c_{16} = c_{25} = c_{26} = c_{35} = c_{36} = c_{45} = c_{46} = 0$$

which shows that there is a plane of symmetry.

2.6.1 Modified Cowin-Mehrabadi Theorems

Mehrabadi and Cowin [29] have shown that only the last two conditions, that is, (2.54) and (2.55) are necessary and sufficient for **n** to be a plane of symmetry. Though conditions (2.52) and (2.55) or (2.53) and (2.55) are also necessary and sufficient conditions for **n** to be a plane of symmetry. Ting [41] has therefore modified the Cowin-Mehrabadi Theorem 2.2, whose statement is given as

Theorem 2.3. An anisotropic elastic material with given elastic stiffnesses c_{ijkl} has a plane of symmetry if and only if **n** is an eigenvector of (i) $Q(\mathbf{n})$ and $Q(\mathbf{m})$, (ii) U and $Q(\mathbf{m})$, or (iii) V and $Q(\mathbf{m})$. The vector **n** is normal to the plane of symmetry while **m** is any vector on the plane of symmetry.

But it is not suitable to determine **n** by Theorem 2.3, because the matrix $Q(\mathbf{m})$ depends on **m** which, in turns, depends on **n**. Therefore Ting [41] has stated another Theorem which is more useful for determining **n**.

Theorem 2.4. An anisotropic elastic material has a plane of symmetry if and only if the normal n to the plane of symmetry is a common eigenvector of \mathbf{U} and \mathbf{V} and satisfies

$$c_{ijkl}m_in_jn_kn_l = 0 (2.63)$$

$$c_{ijkl}m_im_jm_kn_l = 0 (2.64)$$

for any two independent vectors $m^{(\alpha)}(\alpha = 1, 2)$ on the plane of symmetry that don't form an angle a multiple of $\frac{\pi}{3}$.

2.6.2 Generalized Cowin-Mehrabadi Theorems

Ting [30] has generalized Cowin-Mehrabadi Theorem 2.2 in the form of several simplified versions. He has shown that there is no need to satisfy (2.55) for any **m**. In the following consecutive Theorems we will see the different cases of Ting's generalization of Cowin-Mehrabadi Theorem 2.2 :

Theorem 2.5. A necessary and sufficient condition for \mathbf{n} to be normal to a symmetry plane is that \mathbf{n} be an eigenvector of \mathbf{U} , \mathbf{V} , $Q(\mathbf{n})$ and $Q(\mathbf{m})$ for any one \mathbf{m} .

Theorem 2.6. A necessary and sufficient condition for \mathbf{n} to be normal to a symmetry plane is that \mathbf{n} be an eigenvector of \mathbf{U} , \mathbf{V} , and $Q(\mathbf{m})$ for any two distinct \mathbf{m} .

Theorem 2.7. A necessary and sufficient condition for \mathbf{n} to be normal to a symmetry plane is that \mathbf{n} be an eigenvector of \mathbf{U} , $Q(\mathbf{n})$, and $Q(\mathbf{m})$ for any two distinct \mathbf{m} .

Theorem 2.8. A necessary and sufficient condition for \mathbf{n} to be normal to a symmetry plane is that \mathbf{n} be an eigenvector of \mathbf{V} , $Q(\mathbf{n})$, and $Q(\mathbf{m})$ for any two distinct nonorthogonal \mathbf{m} .

Theorem 2.9. A necessary and sufficient condition for \mathbf{n} to be normal to a symmetry plane is that \mathbf{n} be an eigenvector of \mathbf{U} , \mathbf{V} or $\mathbf{Q}(\mathbf{n})$ and any eigenvector of $\mathbf{Q}(\mathbf{m})$ for any three distinct \mathbf{m} .

2.6.3 Cowin-Mehrabadi Theorem for an axis of symmetry

A vector, **p**, is called an *n*-fold axis of rotation or an axis of symmetry, A_n if a crystal is invariant with respect to rotation through an angle $\frac{2\pi}{n}$. The tensor **Q** associated with rotation of a rigid body about an axis **p** by an angle θ is given by

$$\mathbf{Q} = \mathbf{I} + \sin\theta \,\mathbf{P} + (1 - \cos\theta) \,\mathbf{P}^2,\tag{2.65}$$

where the tensor $\mathbf{P} = (P_{ij})$ is defined as $P_{ij} = -\varepsilon_{ijk}p_k$ and \mathbf{I} denotes the unit tensor δ_{ij} [42, 43]. Ahmad [31] has used the above properties to show that a vector parallel to

an axis of symmetry must also satisfy the four conditions, (2.52)-(2.55) of the Cowin-Mehrabadi Theorem. In the following Theorem, he has shown that **p** shares with **n** three conditions, (2.52)-(2.55) out of four given in Theorem 2.2.

Theorem 2.10. A necessary condition for a vector \mathbf{p} to be an axis of symmetry is that it is a common eigenvector of \mathbf{U} , \mathbf{V} and $\mathbf{W}(\mathbf{p})$ as defined in theorem 2.2.

Ahmad [31] has also shown that an axis of rotational symmetry is normal to the plane of symmetry except in the case of trigonal materials. This result can be seen in the following Theorem

Theorem 2.11. A necessary and sufficient condition for an axis of symmetry A_n to be a normal to a plane of symmetry is that n be an even integer i.e n = 2, 4 or 6. Thus A_3 is the only axis of symmetry which is not normal to the plane of symmetry.

If we want to verify whether or not a vector is normal to a plane of symmetry, we need to satisfy the four conditions (see Theorems 2.2-2.9). On the other hand if we want to verify whether or not a vector is an axis of symmetry, is relatively simple. We can observe this in the following Theorem [31].

Theorem 2.12. A sufficient condition for a vector \mathbf{p} to be an axis of symmetry is that it is a common eigenvector of \mathbf{U} and \mathbf{V} corresponding to a nondegenerate eigenvalue.

2.7 Piezoelectricity

Piezoelectricity is a property of materials which converts mechanical energy and electrical energy into one another. If a mechanical force is applied to a solid material and it becomes electrically polarized and if an electric field is applied, it becomes mechanically deformed, the solid is said to be piezoelectric. The former effect is called direct effect and the later one is called inverse effect. The third order piezoelectric tensor can be emerged from the following relation (see [44, 45])

$$D = eS + \varepsilon E \to D_i = e_{ijk}S_{jk} + \varepsilon_{ij}E_j, \qquad (2.66)$$

where **D** is the electric displacement, **E** is the electric field vector, **e** is the third order tensor of piezoelectricity or piezoelectric tensor and ε is the second order dielectric permittivity tensor at null strain field. The piezoelectric constants e_{ijk} relate changes of displacement D_i to strain S_{jk} in the solid provided the electric field held constant, so that

$$e_{ijk} = \frac{\partial D_i}{\partial S_{jk}}|_E.$$
(2.67)

piezoelectric constants e_{ijk} can be expressed in units of C/m^2 . As we know that the strain tensor is symmetric, i.e., $S_{jk} = S_{kj}$, therefore the piezoelectric tensor e_{ijk} is symmetric with respect to the last two indices j and k, so that

$$e_{ijk} = e_{ikj},\tag{2.68}$$

which reduces the number of independent components from 27 to 18. Indeed the last two indices j and k, form a pair which can only take six distinct values represented by the number α . These are numbered 1 to 6 as follows:

$$(11) \leftrightarrow 1, (22) \leftrightarrow 2, (33) \leftrightarrow 3, (23) \leftrightarrow 4, (13) \leftrightarrow 5, (12) \leftrightarrow 6.$$

Thus

$$e_{i\alpha} = e_{ijk}, i = 1, 2, 3, \ \alpha = (j, k) = 1, 2, ..., 6.$$
 (2.69)

Then the matrix form of the piezoelectric tensor is

$$(e_{i\alpha}) = \begin{pmatrix} e_{11} & e_{12} & e_{13} & e_{14} & e_{15} & e_{16} \\ e_{21} & e_{22} & e_{23} & e_{24} & e_{25} & e_{26} \\ e_{31} & e_{32} & e_{33} & e_{34} & e_{35} & e_{36} \end{pmatrix}.$$
 (2.70)

2.7.1 Effect of material symmetry on piezoelectric constants

The number of independent components of piezoelectric tensor (piezoelectric constants) can be further reduced if the crystal possesses one or more symmetry elements. The transformation associated with inversion in a center of symmetry has the matrix representation

$$(Q_{ij}) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$
 (2.71)

Invariance under this transformation leads to the vanishing of every component of a third rank tensor, because

$$e_{ijk} = Q_{il}Q_{jm}Q_{kn}e_{lmn}$$

or

$$e_{ijk} = (-1)^3 e_{ijk}$$

or

$$e_{ijk} = 0.$$

Thus there is no piezoelectricity in any of the centrosymmetric crystals.

A material is said to have *point symmetry group* m if it possesses a single plane of symmetry M. We choose the coordinate axes so that the x_3 -axis is normal to M. The transformation matrix associated with the reflection in M is

$$(Q_{ij}) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$
 (2.72)

A tensor, T_{ij} of rank 2, associated with the material will satisfy the equation

$$T_{ij} = Q_{ip}Q_{jq}T_{pq},$$

with the result that any component with the subscript 3 appearing once will vanish. Thus

$$(T_{ij}) = \begin{pmatrix} T_{11} & T_{12} & 0 \\ T_{21} & T_{22} & 0 \\ 0 & 0 & T_{33} \end{pmatrix}$$
(2.73)

Same reasoning applied to the piezoelectric tensor e_{ijk} indicates that any component having one or three indices equal to 3 must vanish. Making use of the symmetry in the last two indices i.e. $e_{ijk} = e_{ikj}$, we can use the two index notation to write the matrix representation for the tensor as follows

$$(e_{i\alpha}) = \begin{pmatrix} e_{11} & e_{12} & e_{13} & 0 & 0 & e_{16} \\ e_{21} & e_{22} & e_{23} & 0 & 0 & e_{26} \\ 0 & 0 & 0 & e_{34} & e_{35} & 0 \end{pmatrix}$$
(2.74)

where $e_{13} = e_{133}$, $e_{34} = e_{323} = e_{332}$ etc. In (2.74) we follow the usual convention that Latin indices take values 1, 2, 3 and Greek indices take values 1, ..., 6.

A crystal which is symmetric with respect to rotation through an angle π is said to have

the point symmetry group 2. With the x_3 -axis chosen parallel to the axis of symmetry, the piezoelectric tensor for this crystal has the following representation [46, 47]

$$(e_{i\alpha}) = \begin{pmatrix} 0 & 0 & 0 & e_{14} & e_{15} & 0 \\ 0 & 0 & 0 & e_{24} & e_{25} & 0 \\ e_{31} & e_{32} & e_{33} & 0 & 0 & e_{36} \end{pmatrix}.$$
 (2.75)

Similarly, for class 222, we have

$$(e_{i\alpha}) = \begin{pmatrix} 0 & 0 & 0 & e_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & e_{25} & 0 \\ 0 & 0 & 0 & 0 & 0 & e_{36} \end{pmatrix},$$
(2.76)

for class 2mm,

$$(e_{i\alpha}) = \begin{pmatrix} 0 & 0 & 0 & e_{15} & 0 \\ 0 & 0 & 0 & e_{24} & 0 & 0 \\ e_{31} & e_{32} & e_{33} & 0 & 0 & 0 \end{pmatrix}$$
(2.77)

and for classes 4 and 6,

$$(e_{i\alpha}) = \begin{pmatrix} 0 & 0 & 0 & e_{14} & e_{15} & 0 \\ 0 & 0 & 0 & e_{15} & -e_{14} & 0 \\ e_{31} & e_{32} & e_{33} & 0 & 0 & 0 \end{pmatrix}.$$
 (2.78)

The matrix forms of piezoelectric tensor for the remaining crystal classes (out of 32) can be found in [47].

2.8 Young's modulus

Young's modulus $E(\mathbf{n})$ for an elastic material is the ratio of the uniaxial stress applied along the direction of a unit vector \mathbf{n} to the longitudinal strain in the direction \mathbf{n} .

If $\sigma_{11} \neq 0$ and all other components vanish. For this Generalized Hooke's law gives us

$$\varepsilon_{11} = s_{1111}\sigma_{11}$$
$$= s_{11}\sigma_{11}$$

This implies that

Young's modulus
$$=$$
 $\frac{\sigma_{11}}{\varepsilon_{11}} = \frac{1}{s_{11}}$ (2.79)

If we apply uniaxial stress $\sigma n_i n_j$ in an arbitrary direction specified by a unit vector **n** then we can write

$$\sigma_{ij} = \sigma n_i n_j$$

This will create a strain in the material. The component of strain tensor ε_{ij} in the direction **n** is

$$\varepsilon_{ij}n_inj$$
Young's modulus = $E(\mathbf{n}) = \frac{\sigma}{\varepsilon_{ij}n_inj} = \frac{\sigma}{\sigma s_{ijkl}n_in_jn_kn_l}$

$$E(\mathbf{n}) = \frac{1}{s_{ijkl}n_in_jn_kn_l}.$$
(2.80)

For convenience, we usually take the reciprocal of $E(\mathbf{n})$ as

$$\frac{1}{E(\mathbf{n})} = s_{ijkl} n_i n_j n_k n_l. \tag{2.81}$$

2.8.1 Expression of Young's modulus for general anisotropic (triclinic) materials

Using $s_{\alpha\beta}$ as the contracted notation of s_{ijkl} the 6×6 matrix $s_{\alpha\beta}$ is symmetric. The 6×6 matrix for elastic compliances, $s_{\alpha\beta}$ for general anisotropic (*triclinic*) materials has the form

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

$$(2.82)$$

The full expression of Eq.(2.81) becomes

$$\frac{1}{E(\mathbf{n})} = s_{11}n_1^4 + s_{22}n_2^4 + s_{33}n_3^4 + (s_{44} + 2s_{23})n_2^2n_3^2 + (s_{55} + 2s_{13})n_3^2n_1^2 + (s_{66} + 2s_{12})n_1^2n_2^2 + 2n_2n_3[(s_{14} + s_{56})n_1^2 + s_{24}n_2^2 + s_{34}n_3^2] + 2n_3n_1[s_{15}n_1^2 + (s_{25} + s_{46})n_2^2 + s_{35}n_3^2] + 2n_1n_2[s_{16}n_1^2 + s_{26}n_2^2 + (s_{36} + s_{45})n_3^2]$$
(2.83)

This expression is same to that obtained by Ting [48–50]. The expressions of $\frac{1}{E(\mathbf{n})}$ for a particular class of anisotropic materials can be obtained from this expression by using corresponding matrix of compliances in each case. The following is an example for cubic materials.

2.8.2 Expression of Young's modulus for cubic materials

The 6×6 matrix of elastic compliances, $s_{\alpha\beta}$ for cubic elastic materials has the form

$$s = \begin{pmatrix} s_{11} & s_{12} & s_{12} & 0 & 0 & 0\\ s_{12} & s_{11} & s_{12} & 0 & 0 & 0\\ s_{12} & s_{12} & s_{11} & 0 & 0 & 0\\ 0 & 0 & 0 & s_{44} & 0 & 0\\ 0 & 0 & 0 & 0 & s_{44} & 0\\ 0 & 0 & 0 & 0 & 0 & s_{44} \end{pmatrix}$$
(2.84)

therefore for cubic materials Eq.(2.83) reduces to

$$\frac{1}{E(\mathbf{n})} = s_{11}n_1^4 + s_{11}n_2^4 + s_{11}n_3^4 + (s_{44} + 2s_{12})n_2^2n_3^2 + (s_{44} + 2s_{12})n_3^2n_1^2 + (s_{44} + 2s_{12})n_1^2n_2^2$$

$$= s_{11}(n_1^4 + n_2^4 + n_3^4) + (s_{44} + 2s_{12})(n_2^2n_3^2 + n_3^2n_1^2 + n_1^2n_2^2)$$

$$= s_{11}(n_1^2 + n_2^2 + n_3^2)^2 - 2s_{11}(n_2^2n_3^2 + n_3^2n_1^2 + n_1^2n_2^2)$$

$$+ (s_{44} + 2s_{12})(n_2^2n_3^2 + n_3^2n_1^2 + n_1^2n_2^2)$$
(2.85)

Chapter 3

Eigenvectors of a rotation matrix

If a tensor is invariant under rotation about a fixed axis, the matrices representing the tensor and the rotation commute with each other. The two matrices have common eigenvectors, therefore a knowledge of eigenvectors of the rotation matrix provides us with a fair amount of information about eigenvectors of the tensor. In this chapter, we apply this result to derive familiar representations of a transversely isotropic tensor of rank 2 and the elasticity tensor possessing tetragonal symmetry. The assumption of transverse isotropy immediately leads to the conclusion that the tensor must be diagonal with two elements equal. Then, we apply this result to the elasticity tensor possessing an axis of tetragonal symmetry and obtain the classical matrix representation of the tensor. Representation of the elasticity tensor belonging to a particular symmetry class can be achieved in an elegant manner. We use this theory to obtain a partitioning of the elasticity tensor into sets which constitute an associative algebra [32]. This work also reproduces eigenspaces found by Bona et al. [33,34] in their characterization of the symmetry classes of elasticity tensors. These examples are an indication of the power of Mehrabadi-Cowin formalism [11] to approach classical results from a new perspective.

In this chapter, we shall make use of a well-known result of linear algebra which states that if two Hermitian matrices commute then they can be simultaneously diagonalized. This means that a set of orthonormal vectors exists, every member of which, is a *common* eigenvector of both matrices.

3.1 Eigenvectors of commuting matrices

We first apply Theorem 2.1 to find the eigenvectors of a transversely isotropic tensor of rank 2 and then apply it to find the same to fourth rank elasticity tensors of isotropic materials and anisotropic materials of different classes.

3.1.1 Transversely isotropic tensor of rank 2

As an *application* of Theorem 2.1, consider a symmetric tensor T_{ij} which can be represented by the matrix

$$T = \begin{pmatrix} T_{11} & T_{12} & T_{13} \\ T_{12} & T_{22} & T_{23} \\ T_{13} & T_{23} & T_{33} \end{pmatrix}$$
(3.1)

The rotation matrix representing a rotation through an angle θ , about x_3 -axis is

$$Q = \begin{pmatrix} \cos\theta & \sin\theta & 0\\ -\sin\theta & \cos\theta & 0\\ 0 & 0 & 1 \end{pmatrix}$$
(3.2)

Eigenvalues of the matrix Q are

$$1, e^{i\theta}, e^{-i\theta}$$

and the corresponding eigenvectors of Q are

$$\frac{1}{\sqrt{2}}(1,i,0)^T, \frac{1}{\sqrt{2}}(1,-i,0)^T \text{ and } (0,0,1)^T,$$

where, T denotes the transpose. Suppose the tensor T_{ij} possesses transverse isotropy about x_3 -axis i.e. it is invariant with respect to arbitrary rotations about the x_3 -axis. This implies $T = QTQ^{-1}$ or TQ = QT, hence the matrix (3.1) has eigenvectors given in (3.2). Since $(1, i, 0)^T = (1, 0, 0)^T + i(0, 1, 0)^T$, it follows that both $(1, 0, 0)^T$ and $(0, 1, 0)^T$ are eigenvectors of the matrix T belonging to the same eigenvalue while the third eigenvector is $(0, 0, 1)^T$. Thus all eigenvectors of T are found without any appeal to its components. Let the three eigenvectors of the tensor T along with their eigenvalues, be of the following form

$$\lambda_1, v_1 = (1, 0, 0)^T,$$

 $\lambda_2 = \lambda_1, v_2 = (0, 1, 0)^T,$
 $\lambda_3, v_3 = (0, 0, 1)^T.$

Since v_1 and v_2 are eigenvectors belonging to an eigenvalue, λ_1 , say, that is, we have

$$T v_1 = \lambda_1 v_1$$
 and $T v_2 = \lambda_1 v_2$

that is,

and

$$\begin{pmatrix} T_{11} & T_{12} & T_{13} \\ T_{12} & T_{22} & T_{23} \\ T_{13} & T_{23} & T_{33} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \lambda_1 \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$
$$\begin{pmatrix} T_{11} & T_{12} & T_{13} \\ T_{12} & T_{22} & T_{23} \\ T_{13} & T_{23} & T_{33} \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = \lambda_1 \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}.$$

This implies that

$$T_{11} = \lambda_1, T_{12} = T_{13} = 0$$
 and $T_{12} = T_{13} = 0, T_{22} = \lambda$.

Hence $T_{11} = T_{22}$.

Similarly,

$$T v_3 = \lambda_3 v_3$$

that is,

$$\begin{pmatrix} T_{11} & T_{12} & T_{13} \\ T_{12} & T_{22} & T_{23} \\ T_{13} & T_{23} & T_{33} \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = \lambda_3 \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

implies that

$$T_{13} = T_{23} = 0$$
 and $T_{33} = \lambda_3$.

We have recovered the well-known matrix representation for a transversely isotropic tensor of rank 2 [40], 7 ١

$$\begin{pmatrix} T_{11} & 0 & 0 \\ 0 & T_{11} & 0 \\ 0 & 0 & T_{33} \end{pmatrix}.$$

3.1.2**Tetragonal symmetry**

We apply Theorem 2.1 to the elasticity tensor corresponding to a material possessing tetragonal symmetry. For this we consider the rotation about x_3 -axis through an angle θ , which is represented by the following matrix

$$\mathbf{Q} = \begin{pmatrix} \cos\theta & \sin\theta & 0\\ -\sin\theta & \cos\theta & 0\\ 0 & 0 & 1 \end{pmatrix},$$

the corresponding 6D matrix (see section 2.3)

1

$$\hat{\mathbf{Q}} = \hat{\mathbf{Q}}(\theta) = \begin{pmatrix} \cos^2 \theta & \sin^2 \theta & 0 & 0 & 0 & -\sqrt{2} \sin \theta \cos \theta \\ \sin^2 \theta & \cos^2 \theta & 0 & 0 & 0 & \sqrt{2} \sin \theta \cos \theta \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & \cos \theta & -\sin \theta & 0 \\ 0 & 0 & 0 & \sin \theta & \cos \theta & 0 \\ -\sqrt{2} \sin \theta \cos \theta & \sqrt{2} \sin \theta \cos \theta & 0 & 0 & \cos^2 \theta - \sin^2 \theta \end{pmatrix}$$

For tetragonal materials, we have $\theta = \frac{2\pi}{4}$, so that the above matrix becomes

$$\hat{\mathbf{Q}}(\frac{2\pi}{4}) = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 \end{pmatrix}$$

.

The matrix $\hat{c}_{\alpha\beta}$ for tetragonal material commutes with the matrix $\hat{Q}(\frac{2\pi}{4})$. Eigenvalues γ_i of the matrix $\hat{Q}(\frac{2\pi}{4})$ are

$$\gamma_1 = \gamma_2 = 1, \ \gamma_3 = \gamma_4 = -1, \gamma_5 = i, \ \gamma_6 = -i$$

and the corresponding eigenvectors $u_i, i = 1, .., 6$, of $\hat{Q}(\frac{2\pi}{4})$ are

$$u_{1} = (0, 0, 1, 0, 0, 0)^{T},$$

$$u_{2} = (1, 1, 0, 0, 0, 0)^{T},$$

$$u_{3} = (0, 0, 0, 0, 0, 0, 1)^{T},$$

$$u_{4} = (-1, 1, 0, 0, 0, 0)^{T},$$

$$u_{5} = (0, 0, 0, i, 1, 0)^{T},$$

$$u_{6} = (0, 0, 0, -i, 1, 0)^{T}.$$

From the pair of eigenvectors u_1 and u_2 , we deduce the existence of an eigenvector of $\hat{c}_{\alpha\beta}$, of the form

$$a_1u_1 + a_2u_2 = (a_2, a_2, a_1, 0, 0, 0)^T = a_2(1, 1, \frac{a_1}{a_2}, 0, 0, 0)^T$$

Thus we can take $v_1 = (1, 1, a, 0, 0, 0)^T$. An orthogonal vector belonging to the same eigenvalue can be taken as $v_2 = (a, a, -2, 0, 0, 0)^T$. Similarly from the pair of eigenvectors u_3 and u_4 , we can write

$$a_3u_3 + a_4u_4 = (-a_4, a_4, 0, 0, 0, a_3)^T = -a_4(1, -1, 0, 0, 0, \frac{-a_3}{a_4})^T.$$

We may take $v_3 = (1, -1, 0, 0, 0, b)^T$ and as an orthogonal vector belonging to the same eigenvalue we can take $v_4 = (b, -b, 0, 0, 0, -2)^T$. The eigenvectors u_5 and u_6 can be written as

$$u_5 = (0, 0, 0, 0, 1, 0)^T + i (0, 0, 0, 1, 0, 0)^T$$
 and
 $u_6 = (0, 0, 0, 0, 1, 0)^T - i(0, 0, 0, 1, 0, 0)^T$,

respectively. From this we conclude that $\hat{c}_{\alpha\beta}$ will have a *degenerate* eigenvalue with eigenvectors $v_5 = (0, 0, 0, 0, 1, 0)^T$ and $v_6 = (0, 0, 0, 1, 0, 0)^T$. Thus the six eigenvectors of an arbitrary tensor possessing tetragonal symmetry, along with their eigenvalues, are of the

following form

$$\lambda_{1}, v_{1} = (1, 1, a, 0, 0, 0)^{T},$$

$$\lambda_{2}, v_{2} = (a, a, -2, 0, 0, 0)^{T},$$

$$\lambda_{3}, v_{3} = (1, -1, 0, 0, 0, b)^{T},$$

$$\lambda_{4}, v_{4} = (b, -b, 0, 0, 0, -2)^{T},$$

$$\lambda_{5}, v_{5} = (0, 0, 0, 0, 1, 0)^{T},$$

$$\lambda_{6} = \lambda_{5}, v_{6} = (0, 0, 0, 1, 0, 0)^{T}.$$
(3.3)

Bona et al. [33, Eq. 39] found the above representation by a different method. The vectors v_i , i = 1, ..., 6 are mutually orthogonal. The reason for the first four eigenvalues being distinct will be given later. Multiply the vectors by suitable constants in order to normalize them. Denote the *orthonormal* vectors by w_i , i = 1, ..., 6. The *spectral decomposition* of the matrix is given by

$$\hat{c} = \sum_{i=1}^{6} \lambda_i w_i w_i^T \tag{3.4}$$

The above representation contains two parameters a, b and five eigenvalues. These are the seven parameters required to completely specify a tensor possessing tetragonal symmetry. However in a coordinate transformation the eigenvalues remain invariant and only a and b will change.

We shall now use the eigenvectors $v_1, ..., v_6$ to deduce the classical 6×6 matrix representation for an elasticity tensor having tetragonal symmetry. Since v_5 and v_6 are both eigenvectors of $\hat{c}_{\alpha\beta}$ belonging to the same eigenvalue, it follows that

$$\hat{c} v_5 = \lambda_5 v_5$$

$$\begin{pmatrix} \hat{c}_{11} & \hat{c}_{12} & \hat{c}_{13} & \hat{c}_{14} & \hat{c}_{15} & \hat{c}_{16} \\ \hat{c}_{12} & \hat{c}_{22} & \hat{c}_{23} & \hat{c}_{24} & \hat{c}_{25} & \hat{c}_{26} \\ \hat{c}_{13} & \hat{c}_{23} & \hat{c}_{33} & \hat{c}_{34} & \hat{c}_{35} & \hat{c}_{36} \\ \hat{c}_{14} & \hat{c}_{24} & \hat{c}_{34} & \hat{c}_{44} & \hat{c}_{45} & \hat{c}_{46} \\ \hat{c}_{15} & \hat{c}_{25} & \hat{c}_{35} & \hat{c}_{45} & \hat{c}_{55} & \hat{c}_{56} \\ \hat{c}_{16} & \hat{c}_{26} & \hat{c}_{36} & \hat{c}_{46} & \hat{c}_{56} & \hat{c}_{66} \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} = \lambda_5 \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}$$

$$\hat{c}_{15} = \hat{c}_{25} = \hat{c}_{25} = \hat{c}_{25} = \hat{c}_{56} = 0, \ \hat{c}_{55} = \lambda_5$$

and

$$\hat{c} \ v_{6} = \lambda_{5} v_{6}$$

$$\begin{pmatrix} \hat{c}_{11} & \hat{c}_{12} & \hat{c}_{13} & \hat{c}_{14} & \hat{c}_{15} & \hat{c}_{16} \\ \hat{c}_{12} & \hat{c}_{22} & \hat{c}_{23} & \hat{c}_{24} & \hat{c}_{25} & \hat{c}_{26} \\ \hat{c}_{13} & \hat{c}_{23} & \hat{c}_{33} & \hat{c}_{34} & \hat{c}_{35} & \hat{c}_{36} \\ \hat{c}_{14} & \hat{c}_{24} & \hat{c}_{34} & \hat{c}_{44} & \hat{c}_{45} & \hat{c}_{46} \\ \hat{c}_{15} & \hat{c}_{25} & \hat{c}_{35} & \hat{c}_{45} & \hat{c}_{55} & \hat{c}_{56} \\ \hat{c}_{16} & \hat{c}_{26} & \hat{c}_{36} & \hat{c}_{46} & \hat{c}_{56} & \hat{c}_{66} \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} = \lambda_{5} \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$$

$$\hat{c}_{14} = \hat{c}_{24} = \hat{c}_{34} = \hat{c}_{45} = \hat{c}_{46} = 0, \ \hat{c}_{44} = \lambda_{5}.$$

Which implies that $\hat{c}_{44} = \hat{c}_{55}$. Since v_1 is an eigenvector belonging to an eigenvalue, λ_1 , say, that is, we have

$$\hat{c} v_{1} = \lambda_{1} v_{1}$$

$$\begin{pmatrix} \hat{c}_{11} & \hat{c}_{12} & \hat{c}_{13} & \hat{c}_{14} & \hat{c}_{15} & \hat{c}_{16} \\ \hat{c}_{12} & \hat{c}_{22} & \hat{c}_{23} & \hat{c}_{24} & \hat{c}_{25} & \hat{c}_{26} \\ \hat{c}_{13} & \hat{c}_{23} & \hat{c}_{33} & \hat{c}_{34} & \hat{c}_{35} & \hat{c}_{36} \\ \hat{c}_{14} & \hat{c}_{24} & \hat{c}_{34} & \hat{c}_{44} & \hat{c}_{45} & \hat{c}_{46} \\ \hat{c}_{15} & \hat{c}_{25} & \hat{c}_{35} & \hat{c}_{45} & \hat{c}_{55} & \hat{c}_{56} \\ \hat{c}_{16} & \hat{c}_{26} & \hat{c}_{36} & \hat{c}_{46} & \hat{c}_{56} & \hat{c}_{66} \end{pmatrix} \begin{pmatrix} 1 \\ 1 \\ 1 \\ a \\ 0 \\ 0 \\ 0 \end{pmatrix} = \lambda_{1} \begin{pmatrix} 1 \\ 1 \\ a \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

$$\hat{c}_{11} + \hat{c}_{12} + \hat{c}_{13} \ a = \lambda_1,$$

$$\hat{c}_{12} + \hat{c}_{22} + \hat{c}_{23} \ a = \lambda_1,$$

$$\hat{c}_{13} + \hat{c}_{23} + \hat{c}_{33} \ a = \lambda_1 a,$$

$$\hat{c}_{14} + \hat{c}_{24} + \hat{c}_{34} \ a = 0,$$

$$\hat{c}_{15} + \hat{c}_{25} + \hat{c}_{35} \ a = 0,$$

$$\hat{c}_{16} + \hat{c}_{26} + \hat{c}_{36} \ a = 0.$$
(3.5)

The fourth and fifth equations of (3.5) are trivially satisfied. The first two equations imply

$$(\hat{c}_{11} - \hat{c}_{22}) + (\hat{c}_{13} - \hat{c}_{23}) \ a = 0 \tag{3.6}$$

Similarly, for v_2 , we can write

$$\hat{c} v_2 = \lambda_2 v_2$$

$$\begin{pmatrix} \hat{c}_{11} & \hat{c}_{12} & \hat{c}_{13} & \hat{c}_{14} & \hat{c}_{15} & \hat{c}_{16} \\ \hat{c}_{12} & \hat{c}_{22} & \hat{c}_{23} & \hat{c}_{24} & \hat{c}_{25} & \hat{c}_{26} \\ \hat{c}_{13} & \hat{c}_{23} & \hat{c}_{33} & \hat{c}_{34} & \hat{c}_{35} & \hat{c}_{36} \\ \hat{c}_{14} & \hat{c}_{24} & \hat{c}_{34} & \hat{c}_{44} & \hat{c}_{45} & \hat{c}_{46} \\ \hat{c}_{15} & \hat{c}_{25} & \hat{c}_{35} & \hat{c}_{45} & \hat{c}_{55} & \hat{c}_{56} \\ \hat{c}_{16} & \hat{c}_{26} & \hat{c}_{36} & \hat{c}_{46} & \hat{c}_{56} & \hat{c}_{66} \end{pmatrix} \begin{pmatrix} a \\ a \\ -2 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} = \lambda_2 \begin{pmatrix} a \\ a \\ -2 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

$$\hat{c}_{11}a + \hat{c}_{12}a - 2\hat{c}_{13} = \lambda_2 a,$$

$$\hat{c}_{12}a + \hat{c}_{22}a - 2\hat{c}_{23} = \lambda_2 a,$$

$$\hat{c}_{13}a + \hat{c}_{23}a - 2\hat{c}_{33} = -2\lambda_2,$$

$$\hat{c}_{14}a + \hat{c}_{24}a - 2\hat{c}_{34} = 0,$$

$$\hat{c}_{15}a + \hat{c}_{25}a - 2\hat{c}_{35} = 0,$$

$$\hat{c}_{16}a + \hat{c}_{26}a - 2\hat{c}_{36} = 0.$$
(3.7)

Again the fourth and fifth equations of (3.7) are trivially satisfied. The first two equations imply

$$a(\hat{c}_{11} - \hat{c}_{22}) - 2(\hat{c}_{13} - \hat{c}_{23}) = 0$$
(3.8)

The determinant of the system of equations (3.6) and (3.8) is

$$\begin{vmatrix} 1 & a \\ a & -2 \end{vmatrix} = -(2+a^2) \neq 0,$$

therefore $\hat{c}_{11} = \hat{c}_{22}$ and $\hat{c}_{23} = \hat{c}_{13}$. The last equation of (3.5) combined with the corresponding equation (3.7) yields the system

$$(\hat{c}_{16} + \hat{c}_{26}) + \hat{c}_{36} \ a = 0, \tag{3.9}$$

$$a(\hat{c}_{16} + \hat{c}_{26}) - 2\hat{c}_{36} = 0. ag{3.10}$$

Again the determinant of the system of equations (3.9) and (3.10) is

$$\begin{vmatrix} 1 & a \\ a & -2 \end{vmatrix} = -(2+a^2) \neq 0,$$

therefore $\hat{c}_{16} = -\hat{c}_{26}$ and $\hat{c}_{36} = 0$. We have recovered the well-known matrix representation for an elasticity tensor which possesses an axis of tetragonal symmetry

$$\hat{c} = \begin{pmatrix} \hat{c}_{11} & \hat{c}_{12} & \hat{c}_{13} & 0 & 0 & \hat{c}_{16} \\ \hat{c}_{12} & \hat{c}_{11} & \hat{c}_{13} & 0 & 0 & -\hat{c}_{16} \\ \hat{c}_{13} & \hat{c}_{13} & \hat{c}_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & \hat{c}_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & \hat{c}_{44} & 0 \\ \hat{c}_{16} & -\hat{c}_{16} & 0 & 0 & 0 & \hat{c}_{66} \end{pmatrix}.$$

$$(3.11)$$

Eigenvalues of $\hat{c}_{\alpha\beta}$

Since we know the eigenvectors of the matrix (3.11), finding eigenvalues is an easy task. In order to find the eigenvalues corresponding to the eigenvectors v_1 and v_2 , divide the first equation of (3.5) by the third one, we get

$$\frac{\hat{c}_{11} + \hat{c}_{12} + \hat{c}_{13}a}{2\hat{c}_{13} + \hat{c}_{33}a} = \frac{1}{a}$$
(3.12)

where we have made use of the fact $\hat{c}_{13} = \hat{c}_{23}$. The parameter *a* is found by solving the quadratic equation

$$\hat{c}_{13}a^2 + (\hat{c}_{11} + \hat{c}_{12} - \hat{c}_{33})a - 2\hat{c}_{13} = 0, \qquad (3.13)$$

That is

$$a = \frac{-(\hat{c}_{11} + \hat{c}_{12} - \hat{c}_{33}) \pm \sqrt{(\hat{c}_{11} + \hat{c}_{12} - \hat{c}_{33})^2 + 8\hat{c}_{13}^2}}{2\hat{c}_{13}}$$

Note that

$$\frac{1}{2\hat{c}_{13}} \left\{ -(\hat{c}_{11} + \hat{c}_{12} - \hat{c}_{33}) + \sqrt{(\hat{c}_{11} + \hat{c}_{12} - \hat{c}_{33})^2 + 8\hat{c}_{13}^2} \right\}$$

$$\cdot \frac{1}{2\hat{c}_{13}} \left\{ -(\hat{c}_{11} + \hat{c}_{12} - \hat{c}_{33}) - \sqrt{(\hat{c}_{11} + \hat{c}_{12} - \hat{c}_{33})^2 + 8\hat{c}_{13}^2} \right\}$$

$$= \frac{1}{4\hat{c}_{13}^2} ((\hat{c}_{11} + \hat{c}_{12} - \hat{c}_{33})^2 - (\sqrt{(\hat{c}_{11} + \hat{c}_{12} - \hat{c}_{33})^2 + 8\hat{c}_{13}^2})^2$$

$$= \frac{1}{4\hat{c}_{13}^2} ((\hat{c}_{11} + \hat{c}_{12} - \hat{c}_{33})^2 - (\hat{c}_{11} + \hat{c}_{12} - \hat{c}_{33})^2 - 8\hat{c}_{13}^2)$$

$$= -2,$$

that is, the product of the two roots of (3.13) is -2, independent of the material constants. Now the first pair of equations (3.5) now yields

$$\lambda_{1,2} = \frac{\hat{c}_{11} + \hat{c}_{12} + \hat{c}_{33} \pm \sqrt{(\hat{c}_{11} + \hat{c}_{12} - \hat{c}_{33})^2 + 8\hat{c}_{13}^2}}{2}$$
(3.14)

To simplify it, we define $\tan \alpha$ by means of

$$\hat{c}_{11} + \hat{c}_{12} - \hat{c}_{33} = \sqrt{8}\hat{c}_{13}\tan\alpha$$

then (3.14) simplifies to

$$\lambda_{1,2} = \hat{c}_{33} + \sqrt{2}\hat{c}_{13}(\tan\alpha \pm \sec\alpha)$$
(3.15)

The above expression differs slightly from the one reported in [11, Eq. (5.10)] which reads

$$\lambda_{1,2} = \hat{c}_{33} \pm \sqrt{2}\hat{c}_{13}(\tan\alpha + \sec\alpha)$$

The vectors v_1 and v_2 belong to the eigenvalues obtained from (3.14) by choosing the upper and the lower sign respectively. Similarly, to find the eigenvalues corresponding to the eigenvectors v_3 and v_4 , we can write

$$\hat{c} v_3 = \lambda_3 v_3$$

$$\begin{pmatrix} \hat{c}_{11} & \hat{c}_{12} & \hat{c}_{13} & \hat{c}_{14} & \hat{c}_{15} & \hat{c}_{16} \\ \hat{c}_{12} & \hat{c}_{22} & \hat{c}_{23} & \hat{c}_{24} & \hat{c}_{25} & \hat{c}_{26} \\ \hat{c}_{13} & \hat{c}_{23} & \hat{c}_{33} & \hat{c}_{34} & \hat{c}_{35} & \hat{c}_{36} \\ \hat{c}_{14} & \hat{c}_{24} & \hat{c}_{34} & \hat{c}_{44} & \hat{c}_{45} & \hat{c}_{46} \\ \hat{c}_{15} & \hat{c}_{25} & \hat{c}_{35} & \hat{c}_{45} & \hat{c}_{55} & \hat{c}_{56} \\ \hat{c}_{16} & \hat{c}_{26} & \hat{c}_{36} & \hat{c}_{46} & \hat{c}_{56} & \hat{c}_{66} \end{pmatrix} \begin{pmatrix} 1 \\ -1 \\ 0 \\ 0 \\ 0 \\ b \end{pmatrix} = \lambda_3 \begin{pmatrix} 1 \\ -1 \\ 0 \\ 0 \\ 0 \\ b \end{pmatrix}$$

$$\hat{c}_{11} - \hat{c}_{12} + \hat{c}_{16}b = \lambda_3,$$

$$\hat{c}_{12} - \hat{c}_{22} + \hat{c}_{26}b = -\lambda_3,$$

$$\hat{c}_{13} - \hat{c}_{23} + \hat{c}_{36}b = 0,$$

$$\hat{c}_{14} - \hat{c}_{24} + \hat{c}_{46}b = 0,$$

$$\hat{c}_{15} - \hat{c}_{25} + \hat{c}_{56}b = 0,$$

$$\hat{c}_{16} - \hat{c}_{26} + \hat{c}_{66}b = b\lambda_3.$$
(3.16)

Making use of first and last equation of (3.16), we get

$$\frac{\hat{c}_{11} - \hat{c}_{12} + \hat{c}_{16}b}{2\hat{c}_{16} + \hat{c}_{66}b} = \frac{1}{b}$$
(3.17)

where we have made use of the fact $\hat{c}_{26} = -\hat{c}_{16}$. The parameter *b* is found by solving the quadratic equation

$$\hat{c}_{16}b^2 + (\hat{c}_{11} - \hat{c}_{12} - \hat{c}_{66})b - 2\hat{c}_{16} = 0, \qquad (3.18)$$

That is

$$b = \frac{-(\hat{c}_{11} - \hat{c}_{12} - \hat{c}_{66}) \pm \sqrt{(\hat{c}_{11} - \hat{c}_{12} - \hat{c}_{66})^2 + 8\hat{c}_{16}^2}}{2\hat{c}_{16}}$$

Again the product of the two roots of (3.18) is -2, independent of material constants. The first pair of equations (3.16) now yields

$$\lambda_{3,4} = \hat{c}_{66} + \sqrt{2}\hat{c}_{16}(\tan\beta \pm \sec\beta)$$

where $\hat{c}_{11} - \hat{c}_{12} - \hat{c}_{66} = \sqrt{8}\hat{c}_{16} \tan \beta$, in agreement with eigenvalues reported in [11]. And the eigenvalues corresponding to the eigenvectors v_5 and v_6 are \hat{c}_{44} and \hat{c}_{44} , are exactly the same to those reported in [11].

Degeneracy

Since $v_1 = (1, 1, a, 0, 0, 0)$ and $v_2 = (1, 1, -\frac{2}{a}, 0, 0, 0)$ are both eigenvectors of the matrix (3.11). Assume that both of these eigenvectors have the same corresponding eigenvalue, λ , say. That is,

$$\hat{c} v_1 = \lambda v_1$$
 and $\hat{c} v_2 = \lambda v_2$.

This implies that

$$\hat{c}_{11} + \hat{c}_{12} + \hat{c}_{13} \ a = \lambda,$$

$$\hat{c}_{12} + \hat{c}_{22} + \hat{c}_{23} \ a = \lambda,$$

$$\hat{c}_{13} + \hat{c}_{23} + \hat{c}_{33} \ a = \lambda a,$$
(3.19)

and

$$\hat{c}_{11} + \hat{c}_{12} - \frac{2}{a}\hat{c}_{13} = \lambda,$$

$$\hat{c}_{12} + \hat{c}_{22} - \frac{2}{a}\hat{c}_{23} = \lambda,$$

$$\hat{c}_{13} + \hat{c}_{23} - \frac{2}{a}\hat{c}_{33} = -\frac{2}{a}\lambda.$$
(3.20)

Using the first equations of (3.19) and (3.20),

$$\hat{c}_{13}a + \frac{2}{a}\hat{c}_{13} = 0,$$

 $\hat{c}_{13}(a^2 + 2) = 0,$

Which holds only if $\hat{c}_{13} = 0$. But this condition fails to hold. Therefore the two eigenvalues will be distinct. A similar argument applied to v_3 and v_4 shows that since $\hat{c}_{66} \neq 0$, the corresponding eigenvalues will be distinct. A similar situation prevails in other classes of crystal symmetry. Thus a *degenerate* real eigenvalue of the rotation matrix implies *nondegenerate* eigenvalues of the elasticity tensor. On the other hand we have already observed that a non-degenerate complex eigenvalue of the rotation matrix leads to degeneracy in the elasticity tensor.

3.2 Representation of elasticity tensors

Let the matrix \hat{c} satisfy the following eigenvalue equation

$$\hat{c}v_i = \lambda_i v_i, \ i = 1, \dots, 6.$$

Since \hat{c} is a positive definite symmetric matrix, a set of orthonormal vectors $\{v_i\}_{i=1}^6$ exists and $\lambda_i > 0, i = 1, ..., 6$. Define

c

$$E_i = v_i v_i^T, \text{ no summation on } i, \qquad (3.21)$$

where \hat{c} has the representation

$$\hat{c} = \sum_{i=1}^{6} \lambda_i E_i \tag{3.22}$$

It is easy to see that E_i satisfy

$$E_i E_j = 0, i \neq j \tag{3.23}$$

$$E_i^2 = E_i, \ i = 1, ..., 6 \tag{3.24}$$

$$I = E_1 + \dots + E_6 \tag{3.25}$$

where I denotes the unit matrix of order 6. The representation (3.22) has the merit of reducing the calculation of powers and products of \hat{c} to trivial calculations. For example

$$(\hat{c})^{k} = \sum_{i=1}^{6} \lambda_{i}^{k} E_{i}$$
(3.26)

$$(\hat{c})^{-k} = \sum_{i=1}^{6} \lambda_i^{-k} E_i \tag{3.27}$$

and if

$$\hat{c}_1 = \sum_{i=1}^6 \mu_i E_i, \tag{3.28}$$

then

$$\hat{c}\hat{c}_1 = \sum_{i=1}^6 \lambda_i \mu_i E_i \tag{3.29}$$

Representation (3.22) of a matrix is also useful in defining the logarithm of a matrix,

$$\operatorname{Log} \hat{c} = \sum_{i=1}^{6} \ln \lambda_i v_i v_i^T \tag{3.30}$$

which in turn, may be employed to endow a metric space structure to a class of matrices [56].

Walpole [32] has defined an algebra of fourth-rank tensors and has defined fourth-rank tensors E_i in terms of components of mutually perpendicular unit vectors **a**, **b** and **c**. These tensors, for various crystal classes, are designed in such a manner as to satisfy counterparts of equations (3.23)-(3.25), hence they yield a representation in the form of (3.22). The task is made much easier in the Mehrabadi-Cowin formalism. We utilize the theory of previous section and construct matrices E_i from our knowledge of eigenvectors of the matrix associated with the elasticity tensors pertaining to a particular crystal symmetry.

3.2.1 Cubic materials

The matrix representation \hat{c} of the elasticity tensor for cubic materials has the following form

$$\hat{c} = \begin{pmatrix} \hat{c}_{11} & \hat{c}_{12} & \hat{c}_{12} & 0 & 0 & 0 \\ \hat{c}_{12} & \hat{c}_{11} & \hat{c}_{12} & 0 & 0 & 0 \\ \hat{c}_{12} & \hat{c}_{12} & \hat{c}_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & \hat{c}_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & \hat{c}_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & \hat{c}_{44} \end{pmatrix}$$

Let $\lambda_1, \lambda_2, ..., \lambda_6$ be the eigenvalues of \hat{c} . These eigenvalues and the corresponding eigenvectors of \hat{c} can be find as follows

$$\lambda_{1} = \hat{c}_{11} + 2\hat{c}_{12}, v_{1} = \frac{1}{\sqrt{3}} (1, 1, 1, 0, 0, 0)^{T},$$

$$\lambda_{2} = \hat{c}_{11} - \hat{c}_{12}, v_{2} = \frac{1}{\sqrt{6}} (1, 1, -2, 0, 0, 0)^{T},$$

$$\lambda_{3} = \lambda_{2}, v_{3} = \frac{1}{\sqrt{2}} (1, -1, 0, 0, 0, 0)^{T},$$

$$\lambda_{4} = \lambda_{5} = \lambda_{6} = \hat{c}_{44},$$

$$v_{4} = (0, 0, 0, 1, 0, 0)^{T},$$

$$v_{5} = (0, 0, 0, 0, 1, 0)^{T},$$

$$v_{6} = (0, 0, 0, 0, 0, 1)^{T}$$
(3.31)

Equation (3.22) becomes

$$\hat{c} = \lambda_1 E_1 + \lambda_2 (E_2 + E_3) + \lambda_4 (E_4 + E_5 + E_6)$$

= $\lambda_1 F_1 + \lambda_2 F_2 + \lambda_4 F_3$ (3.32)

where

and

The matrices F_1 , F_2 and F_3 are the same as the matrices \hat{J} , \hat{K} and \hat{L} which are the notations of Norris [57] and Walpole [32]. We note that the representation (3.32) of the

tensor \hat{c} , is an invariant representation which characterize the cubic materials.

3.2.2Isotropic materials

For isotropic materials the matrix \hat{c} has the form

,

$$\hat{c} = \begin{pmatrix} \hat{c}_{11} & \hat{c}_{12} & \hat{c}_{12} & 0 & 0 & 0 \\ \hat{c}_{12} & \hat{c}_{11} & \hat{c}_{12} & 0 & 0 & 0 \\ \hat{c}_{12} & \hat{c}_{12} & \hat{c}_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & \hat{c}_{11} - \hat{c}_{12} & 0 & 0 \\ 0 & 0 & 0 & 0 & \hat{c}_{11} - \hat{c}_{12} & 0 \\ 0 & 0 & 0 & 0 & 0 & \hat{c}_{11} - \hat{c}_{12} \end{pmatrix}$$

which is easily seen to have the following eigenvalues

$$\lambda_1 = \hat{c}_{11} + 2\hat{c}_{12}$$

 $\lambda_2 = \lambda_3 = \lambda_4 = \lambda_5 = \lambda_6 = \hat{c}_{11} - \hat{c}_{12},$

and the corresponding eigenvectors v_i , i = 1, ..., 6, are the same as given by (3.31). But the eigenvectors $v_2,...,v_6$ belong to the eigenvalue \hat{c}_{44} which becomes five fold degenerate. Now the matrix \hat{c} has the representation

$$\hat{c} = \lambda_1 F_1 + \lambda_2 F_4 \tag{3.33}$$

where

$$F_{4} = E_{2} + E_{3} + E_{4} + E_{5} + E_{6} = v_{2}v_{2}^{T} + v_{3}v_{3}^{T}v_{4}v_{4}^{T} + v_{5}v_{5}^{T} + v_{6}v_{6}^{T}$$

$$= \frac{1}{3} \begin{pmatrix} 2 & -1 & -1 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 & 0 \\ -1 & -1 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 3 \end{pmatrix}.$$

It can be easily shown that $F_1F_4 = 0$, $F_1^2 = E_1$ and $F_4^2 = F_4$. Also $E_1 + F_4 = I$.

3.2.3 Transversely isotropic materials or hexagonal materials

The elasticity tensor which is invariant under rotation about x_3 -axis, through an arbitrary angle is said to possess transverse isotropy with respect to x_3 -axis. If θ is arbitrary, the matrix $\hat{\mathbf{Q}}$ has the following eigenvalues and eigenvectors

1,
$$(0, 0, 1, 0, 0, 0)^T$$
,
1, $\frac{1}{\sqrt{2}} (1, 1, 0, 0, 0, 0)^T$,
 $e^{-i\theta}, \frac{1}{\sqrt{2}} (0, 0, 0, -i, 1, 0)^T$,
 $e^{i\theta}, \frac{1}{\sqrt{2}} (0, 0, 0, i, 1, 0)^T$,
 $e^{-2i\theta}, \frac{1}{\sqrt{3}} (i, -i, 0, 0, 0, 1)^T$,
 $e^{2i\theta}, \frac{1}{\sqrt{3}} (-i, i, 0, 0, 0, 1)^T$ (3.34)

It is clear that the matrix \hat{c} for transversely isotropic materials or hexagonal materials has the following eigenvectors

$$\lambda_{1}, v_{1} = \frac{1}{\sqrt{2 + a^{2}}} (1, 1, a, 0, 0, 0)^{T},$$

$$\lambda_{2}, v_{2} = \frac{1}{\sqrt{4 + 2a^{2}}} (a, a, -2, 0, 0, 0)^{T},$$

$$\lambda_{3}, v_{3} = \frac{1}{\sqrt{2}} (1, -1, 0, 0, 0, 0)^{T},$$

$$\lambda_{4} = \lambda_{3}, v_{4} = (0, 0, 0, 0, 0, 1)^{T},$$

$$\lambda_{5}, v_{5} = (0, 0, 0, 1, 0, 0)^{T},$$

$$\lambda_{6} = \lambda_{5}, v_{6} = (0, 0, 0, 0, 1, 0)^{T},$$
(3.35)

The above representation is equivalent to Eq. (19) in [33]. Matrix \hat{c} for a transversely isotropic materials or hexagonal materials has the following representation

$$\hat{c} = \lambda_1 E_1 + \lambda_2 E_2 + \lambda_3 (E_3 + E_4) + \lambda_5 (E_5 + E_6)$$
(3.36)

where E_i , i = 1, ..., 6 have been defined in (3.21). Expressions for these matrices can be

written as

From (3.36) it is easy to verify familiar relations between the components of a transversely isotropic tensor or hexagonal tensor. For example, any component c_{ijkl} with an odd number of 1, 2 or 3 vanishes. Moreover

$$\hat{c}_{11} = \hat{c}_{22} = \frac{\lambda_1}{2+a^2} + \frac{\lambda_2 a^2}{4+2a^2} + \frac{1}{2}\lambda_3,$$
$$\hat{c}_{66} = \lambda_3 = \hat{c}_{11} - \hat{c}_{12},$$
$$\hat{c}_{44} = \hat{c}_{55} = \lambda_5,$$
$$\hat{c}_{13} = \hat{c}_{23} = \frac{\lambda_1 a}{2+a^2} - \frac{2\lambda_2 a}{4+2a^2}.$$

Thus we can write the following familiar matrix representation of the elasticity tensor for transversely isotropic materials or hexagonal materials

$$\hat{c} = \begin{pmatrix} \hat{c}_{11} & \hat{c}_{12} & \hat{c}_{13} & 0 & 0 & 0 \\ \hat{c}_{12} & \hat{c}_{11} & \hat{c}_{13} & 0 & 0 & 0 \\ \hat{c}_{13} & \hat{c}_{13} & \hat{c}_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & \hat{c}_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & \hat{c}_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & \hat{c}_{11} - \hat{c}_{12} \end{pmatrix}.$$

3.2.4 Tetragonal materials

We try to find the familiar matrix representation \hat{c} of the elasticity tensor for tetragonal materials, alternatively. For this, let λ_i , i = 1, 2, ...6, be its eigenvalues. For tetragonal materials $\theta = \frac{\pi}{2}$, therefore the matrix $\mathbf{Q}(\frac{\pi}{2})$ and \hat{c} have common eigenvectors. The eigenvectors corresponding to λ_i are as given in (3.3). The tensor \hat{c} has the following representation

$$\hat{c} = \lambda_1 E_1 + \lambda_2 E_2 + \lambda_3 E_3 + \lambda_4 E_4 + \lambda_5 (E_5 + E_6)$$
(3.39)

where E_1 and E_2 are the same as given respectively by (3.37) and (3.38), while rest of the matrices are as follows

,

and

It is easily verified that $E_1 + ... + E_6 = I$ and $E_i E_j = 0, i \neq j$ and $E_i^2 = E_i$. Also the familiar relations between the components of a tensor with tetragonal symmetry (see 3.1.2) are easily verified. For example

$$\begin{aligned} \hat{c}_{11} &= \hat{c}_{22} = \frac{\lambda_1}{2+a^2} + \frac{\lambda_2 a^2}{4+2a^2} + \frac{\lambda_3}{2+b^2} + \frac{\lambda_4 b^2}{4+2b^2}, \\ \hat{c}_{16} &= \frac{\lambda_3 b}{2+b^2} - \frac{\lambda_4 b}{2+b^2} = -\hat{c}_{26}, \\ \hat{c}_{44} &= \hat{c}_{55} = \lambda_5 \end{aligned}$$

Also

$$\hat{c}_{66} = \frac{\lambda_3 b^2}{2+b^2} + \frac{2\lambda_4}{2+b^2}$$

Thus the element \hat{c}_{66} is a weighted average of the eigenvalues λ_3 and λ_4 and will lie between them. Thus we can write the following familiar matrix representation of the elasticity tensor for tetragonal materials

$$\hat{c} = \begin{pmatrix} \hat{c}_{11} & \hat{c}_{12} & \hat{c}_{13} & 0 & 0 & \hat{c}_{16} \\ \hat{c}_{12} & \hat{c}_{11} & \hat{c}_{13} & 0 & 0 & -\hat{c}_{16} \\ \hat{c}_{13} & \hat{c}_{13} & \hat{c}_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & \hat{c}_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & \hat{c}_{44} & 0 \\ \hat{c}_{16} & -\hat{c}_{16} & 0 & 0 & 0 & \hat{c}_{66} \end{pmatrix}$$

3.2.5 Trigonal materials

The matrix \hat{c} representing the elasticity tensor for trigonal materials and the rotation matrix $\hat{Q}\left(\frac{2\pi}{3}\right)$ commute with each other. Therefore both of these matrices have common eigenvectors. The eigenvalues of $\hat{Q}\left(\frac{2\pi}{3}\right)$ are $1, 1, e^{\pm i\theta}, e^{\pm 2i\theta}$. Among these eigenvalues $e^{\pm i\theta} =$

 $\frac{-1\pm i\sqrt{3}}{2}$ and $e^{\pm 2i\theta} = \frac{-1\mp i\sqrt{3}}{2}$ become degenerate. The pairs of eigenvalues and corresponding eigenvectors of the matrix $\hat{Q}(\frac{2\pi}{3})$ are as follow

$$1, (0, 0, 1, 0, 0, 0)^{T},
1, \frac{1}{\sqrt{2}}(1, 1, 0, 0, 0, 0)^{T},
\frac{-1 + i\sqrt{3}}{2}, \frac{1}{2}(i, -i, 0, 0, 0, \sqrt{2})^{T},
\frac{-1 + i\sqrt{3}}{2}, \frac{1}{\sqrt{2}}(0, 0, 0, i, 1, 0)^{T},
\frac{-1 - i\sqrt{3}}{2}, \frac{1}{2}(-i, i, 0, 0, 0, \sqrt{2})^{T},
\frac{-1 - i\sqrt{3}}{2}, \frac{1}{\sqrt{2}}(0, 0, 0, -i, 1, 0)^{T}$$
(3.40)

Let λ_i , i = 1, 2, ..., 6, be the eigenvalues of \hat{c} and v_i , i = 1, 2, ..., 6, be its eigenvectors corresponding to λ_i . The first two eigenvectors of \hat{c} are the same as these in (3.35) i.e.

$$\lambda_1, v_1 = \frac{1}{\sqrt{2+a^2}} (1, 1, a, 0, 0, 0)^T$$
(3.41a)

$$\lambda_2, v_2 = \frac{1}{\sqrt{4+2a^2}} (a, a, -2, 0, 0, 0)^T$$
(3.41b)

To obtain v_3 and v_4 we form a linear combination of the third and fourth vectors of (3.40) i.e.

$$\begin{pmatrix} i \\ -i \\ 0 \\ 0 \\ 0 \\ 0 \\ \sqrt{2} \end{pmatrix} + (c+id) \begin{pmatrix} 0 \\ 0 \\ 0 \\ i \\ 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ -d \\ c \\ \sqrt{2} \end{pmatrix} + i \begin{pmatrix} 1 \\ -1 \\ 0 \\ c \\ d \\ 0 \end{pmatrix}$$

Thus, we can take

$$\lambda_3, v_3 = \frac{1}{\sqrt{2+c^2+d^2}} (1, -1, 0, c, d, 0)^T$$
(3.41c)

$$\lambda_4 = \lambda_3, \quad v_4 = \frac{1}{\sqrt{2 + c^2 + d^2}} (0, 0, 0, -d, c, \sqrt{2})^T$$
 (3.41d)

as a pair of degenerate eigenvectors of \hat{c} . To obtain v_5 and v_6 we form the following linear combination of the last two vectors of (3.40) i.e.

$$\begin{pmatrix} -i \\ i \\ 0 \\ 0 \\ 0 \\ 0 \\ \sqrt{2} \end{pmatrix} - (e - if) \begin{pmatrix} 0 \\ 0 \\ 0 \\ -i \\ 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ f \\ -e \\ \sqrt{2} \end{pmatrix} + i \begin{pmatrix} -1 \\ 1 \\ 0 \\ e \\ f \\ 0 \end{pmatrix},$$

provided that it should yield eigenvectors which are orthogonal to the vectors v_3 as well as v_4 . These vectors will be orthogonal if it satisfy

$$ce + df = 2$$
 and $cf = de$.

This implies that

$$e = \frac{2c}{c^2 + d^2}$$
 and $f = \frac{2d}{c^2 + d^2}$.

Thus the pair of eigenvectors v_5 and v_6 can be written as

$$\lambda_5, v_5 = \frac{\sqrt{c^2 + d^2}}{\sqrt{2c^2 + 2d^2 + 4}} (-1, 1, 0, \frac{2c}{c^2 + d^2}, \frac{2d}{c^2 + d^2}, 0)^T$$
(3.41e)

$$\lambda_6 = \lambda_5, v_6 = \frac{\sqrt{c^2 + d^2}}{\sqrt{2c^2 + 2d^2 + 4}} (0, 0, 0, \frac{2d}{c^2 + d^2}, -\frac{2c}{c^2 + d^2}, \sqrt{2})^T$$
(3.41f)

Thus all eigenvectors of \hat{c} can be expressed in terms of three parameters. The matrix representation of \hat{c} is as follows

$$\hat{c} = \lambda_1 E_1 + \lambda_2 E_2 + \lambda_3 (E_3 + E_4) + \lambda_5 (E_5 + E_6)$$
(3.42)

where E_1 and E_2 are given respectively by (3.37) and (3.38) and
Advantages of new decomposition of elasticity tensor

Throughout this chapter we decomposed matrix representation the elasticity tensor for isotropic and anisotropic materials in a new form. In the following lines, we give some reasons which will show that these new decompositions are convenient:

- (i). For the cubic system, the representation (3.33) of the elasticity tensor \hat{c} contains three parameters, λ_1, λ_2 and λ_4 . These parameters are eigenvalues of the tensor and these are invariant under a coordinate transformation.
- (ii). For a transversely isotropic system, the representation (3.36) of the elasticity tensor \hat{c} contains five parameters, $\lambda_1, \lambda_2, \lambda_3, \lambda_5$ and a. The first four parameters are invariant under a coordinate transformation.
- (iii). For a tetragonal system, the representation (3.39) of the elasticity tensor \hat{c} contains seven parameters, $\lambda_1, \lambda_2, \lambda_3, \lambda_5$, a and b. The first five parameters are invariant under a coordinate transformation.
- (iv). Similarly for a trigonal system, the representation (3.42) of the elasticity tensor \hat{c} contains seven parameters, $\lambda_1, \lambda_2, \lambda_3, \lambda_5, a, c$ and d. The first four parameters are invariant under a coordinate transformation.

The strain energy is defined as

$$W = \frac{1}{2} \sum_{i=1}^{6} \Lambda_i \left| \hat{\mathbf{E}} \cdot \hat{\mathbf{N}}_i \right|^2 \text{ where}(i = 1, 2..., 6), \qquad (3.43)$$

where the vectors $\hat{\mathbf{N}}$ represent the normalized eigenvectors of the six-dimensional matrix \hat{c} , the six eigentensors of strain are denoted by $\hat{\mathbf{E}}$ and Λ_i are the eigenvalues of \hat{c} . Cowin and Yang [16] have shown that this strain energy can be minimized with respect to single strain state, by finding the elastic symmetry with the set of eigenvectors for fixed eigenvalues. They have constructed the matrix representation for elasticity tensor corresponding to the basis $\{\mathbf{N}_i\}_{i=1}^6$ that minimized the strain energy with respect to a single strain state. Instead of this basis, we use the basis $\{\mathbf{v}_i\}_{i=1}^6$ as derived in previous two sections. we will show that the later basis is more general than the previous one. Hence these results of the work done by Cowin and Yang can be treated in a more general manner. First we consider the tetragonal symmetry, where the two principal strains of the strain states are equal [16]. The basis $\{\mathbf{N}_i\}_{i=1}^6$ is

$$\hat{\mathbf{N}}_{1} = \left(\frac{\sin\beta}{\sqrt{2}}, \frac{\sin\beta}{\sqrt{2}}, \cos\beta, 0, 0, 0\right)^{T}, \\
\hat{\mathbf{N}}_{2} = \left(\frac{\cos\beta}{\sqrt{2}}, \frac{\cos\beta}{\sqrt{2}}, -\sin\beta, 0, 0, 0\right)^{T}, \\
\hat{\mathbf{N}}_{3} = \left(\frac{1}{\sqrt{2}}, \frac{-1}{\sqrt{2}}, 0, 0, 0, 0\right)^{T}, \\
\hat{\mathbf{N}}_{4} = (0, 0, 0, 1, 0, 0)^{T}, \\
\hat{\mathbf{N}}_{5} = (0, 0, 0, 0, 1, 0)^{T}, \\
\hat{\mathbf{N}}_{6} = (0, 0, 0, 0, 0, 1)^{T},$$
(3.44)

where β is a parameter. But the basis $\{\mathbf{v}_i\}_{i=1}^6$ for tetragonal symmetry, as derived in section 3.2, can be written as follows

$$v_{1} = \left(\frac{1}{\sqrt{2+a^{2}}}, \frac{1}{\sqrt{2+a^{2}}}, \frac{a}{\sqrt{2+a^{2}}}, 0, 0, 0\right)^{T},$$

$$v_{2} = \left(\frac{a}{\sqrt{4+2a^{2}}}, \frac{a}{\sqrt{4+2a^{2}}}, -\frac{2}{\sqrt{4+2a^{2}}}, 0, 0, 0\right)^{T},$$

$$v_{3} = \left(\frac{1}{\sqrt{2+b^{2}}}, -\frac{1}{\sqrt{2+b^{2}}}, 0, 0, 0, \frac{b}{\sqrt{2+b^{2}}}\right)^{T},$$

$$v_{4} = \left(\frac{b}{\sqrt{4+2b^{2}}}, -\frac{b}{\sqrt{4+2b^{2}}}, 0, 0, 0, -\frac{2}{\sqrt{4+2b^{2}}}\right)^{T},$$

$$v_{5} = (0, 0, 0, 1, 0, 0)^{T},$$

$$v_{6} = (0, 0, 0, 0, 1, 0)^{T}.$$
(3.45)

where a and b are the parameters. If we compare the two bases in (3.44) and (3.45), we can easily see that

$$\hat{\mathbf{N}}_1 = \mathbf{v}_1, \hat{\mathbf{N}}_2 = \mathbf{v}_2, \hat{\mathbf{N}}_4 = \mathbf{v}_6, \hat{\mathbf{N}}_5 = \mathbf{v}_5, \text{ if } a = \sqrt{2} \cot \beta,$$

while

$$\hat{\mathbf{N}}_3 = \mathbf{v}_3$$
 and $\hat{\mathbf{N}}_6 = \mathbf{v}_4$ only if $b = 0$.

But if $b \neq 0$, then these two bases are not the same and therefore the basis $\{\mathbf{v}_i\}_{i=1}^6$ is more general than $\{\mathbf{N}_i\}_{i=1}^6$. By using these basis, the matrix \hat{c} can be expressed in terms of the strain parameters a, b and the eigenvalues $\lambda_i, i = 1, ..., 6$ as in equation (3.39). Next, we consider hexagonal (transverse isotropy) symmetry that admits a basis $\{\mathbf{v}_i\}_{i=1}^6$ containing eigenvectors with two equal principal strains states. The eigenvectors for this symmetry and tetragonal symmetry are the same [16]. They are distinguished only by different eigenvalues. On the other hand, the basis $\{\mathbf{v}_i\}_{i=1}^6$ for hexagonal symmetry can be seen in (3.35), which contains only one parameter a. We can easily see that all the eigenvectors of (3.44) and (3.35) are the same if $a = \sqrt{2} \cot \beta$. The matrix \hat{c} for this case is given by (3.36).

Now for Trigonal symmetry, the basis $\{\mathbf{N}_i\}_{i=1}^6$ used by Cowin and Yang [16] contains the eigenvectors which are not all orthogonal. But if we write it in the following correct form, then the vectors become orthogonal, that is

$$\hat{\mathbf{N}}_{1} = \left(\frac{\sin\beta}{\sqrt{2}}, \frac{\sin\beta}{\sqrt{2}}, \cos\beta, 0, 0, 0\right)^{T}, \\
\hat{\mathbf{N}}_{2} = \left(\frac{\cos\beta}{\sqrt{2}}, \frac{\cos\beta}{\sqrt{2}}, -\sin\beta, 0, 0, 0\right)^{T}, \\
\hat{\mathbf{N}}_{3} = \left(\frac{\cos\gamma}{\sqrt{2}}, -\frac{\cos\gamma}{\sqrt{2}}, 0, \sin\gamma, 0, 0\right)^{T} \\
\hat{\mathbf{N}}_{4} = \left(-\frac{\sin\gamma}{\sqrt{2}}, \frac{\sin\gamma}{\sqrt{2}}, 0, \cos\gamma, 0, 0\right)^{T}, \\
\hat{\mathbf{N}}_{5} = (0, 0, 0, 0, -\cos\gamma, \sin\gamma)^{T}, \\
\hat{\mathbf{N}}_{6} = (0, 0, 0, 0, \sin\gamma, \cos\gamma)^{T},$$
(3.46)

where β and γ are the parameters. The vectors of the basis $\{\mathbf{v}_i\}_{i=1}^6$, for trigonal symmetry are given by (3.41*a*)-(3.41*f*), where the parameters are *a*, *c* and *d*. The comparison of (3.46) with (3.41*a*)-(3.41*f*) gives the following results

$$\hat{\mathbf{N}}_1 = \mathbf{v}_1$$
 and $\hat{\mathbf{N}}_2 = \mathbf{v}_2$, if $a = \sqrt{2} \cot \beta$,

while

$$\hat{\mathbf{N}}_3 = \mathbf{v}_3, \hat{\mathbf{N}}_4 = \mathbf{v}_5, \hat{\mathbf{N}}_5 = \mathbf{v}_6 \text{ and } \hat{\mathbf{N}}_6 = \mathbf{v}_4 \text{ only if } d = 0 \text{ and } c = \sqrt{2} \tan \gamma.$$

But again if $d \neq 0$, the the basis vectors in $\{\mathbf{v}_i\}_{i=1}^6$ are more general than those in the basis $\{\mathbf{N}_i\}_{i=1}^6$. Thus we can get more general form of the problem as discussed above.

Chapter 4

Planes and axes of symmetry

To study the physical properties of anisotropic materials, we use tensors. For instance, the dielectric tensor, ε , of rank two, the piezoelectric tensor, e, of rank three and the elasticity tensor, \mathbf{c} , of rank four. The components of these tensors can be arranged and it is usual to represent it by a matrix. Due to the effect of symmetry with the choice of an axis of rectangular coordinate system, taken to be parallel to the normal of symmetry plane or an axis of symmetry, some of these components vanish and the matrix form consisting of the remaining nonzero components becomes simpler. But if we consider an arbitrary coordinate system, then these components may not vanish and it is not obvious to identify the symmetry class of the elastic materials under consideration. For the identification of plane of symmetry, Cowin and Mehrabadi [28] have proved Theorem 2.2, which is also known as Cowin-Mehrabadi Theorem. The conditions (2.52)-(2.55) of theorem 2.2 were modified by Cowin [29] and has reduced to only two conditions (2.54) and (2.55). Ting [30] has further generalized Cowin-Mehrabadi Theorem and has provided its several cases. Ahmad [31] has proved Cowin-Mehrabadi Theorem for an axis of symmetry. He has also proved Cowin-Mehrabadi Theorem in six dimensions [21]. In this chapter, we provide simple proofs of the necessary and sufficient conditions for the identification of a plane of symmetry or an axis of symmetry in an elastic material. This approach is generalized to a cartesian tensor of arbitrary rank and apply this treatment to find the necessary and sufficient conditions for the existence of a symmetry plane or an axis of symmetry for a piezoelectric material. We also obtain the conditions for the identification of an *n*-fold axis

of symmetry with $n \ge 3$.

This chapter consists of four sections. In section 4.1 we provide simple and short proofs of necessary and sufficient conditions of Theorems 2.2 and 2.10 by searching for invariant directions associated with the elasticity tensor. In case of plane of symmetry, such a direction must be orthogonal to the normal \mathbf{n} whereas in case of axis of symmetry, it must be parallel to the vector \mathbf{p} . In section 4.2, we generalize the approach of section 4.1 to tensors of arbitrary rank and apply it to the third rank piezoelectric tensor to identify the plane of symmetry and do the same in section 4.3 for an axis of symmetry of piezoelectric material. In each of the previous sections the results are illustrated by explicit examples. In section 4.4, we develop the results in the first two sections and generalize them to a tenor of arbitrary rank.

4.1 Simple proofs of necessary conditions

4.1.1 Normal to the plane of symmetry

In an elastic material, suppose a plane of symmetry exists with \mathbf{n} as normal. From (2.34) and (2.35), it is clear that 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. Let us apply transformation (2.34) to \mathbf{n} and \mathbf{m} and denote the transformed vectors with a prime then, (2.35) can be written as

$$\mathbf{n}' = -\mathbf{n} \quad \text{and} \quad \mathbf{m}' = \mathbf{m} \tag{4.1}$$

where **m** is any vector on the plane such that $\mathbf{m} \perp \mathbf{n}$. Conversely, if a vector reverses its direction, it can't have a component in the plane orthogonal to **n**, hence it must be parallel to **n**. Now consider the vectors $U_{ij}n_j = c_{ijkk}n_j$, $V_{ij}n_j = c_{ikjk}n_j$, $W_{ik}(\mathbf{n})n_k = c_{ijkl}n_jn_kn_l$ and $W_{ik}(\mathbf{m})n_k = c_{ijkl}m_jn_km_l$. By using (4.1), these vectors will, respectively, transform

as follows

$$(U_{ij}n_j)' = (c_{ijkk}n_j)' = c'_{ijkk}n'_j, = c_{ijkk}(-n_j) = -c_{ikjj}n_j,$$
(4.2)

$$(V_{ij}n_j)' = (c_{ikjk}n_j)' = c'_{ikjk}n'_j = c_{ikjk}(-n_j) = -c_{ikjk}n_j,$$
(4.3)

$$(W_{ik}(\mathbf{n})n_k)' = (c_{ijkl}n_jn_kn_l)' = c'_{ijkl}n'_jn'_kn'_l$$

= $c_{ijkl}(-n_j)(-n_k)(-n_l) = -c_{ijkl}n_jn_kn_l,$ (4.4)

$$(W_{ik}(\mathbf{m})n_k)' = (c_{ijkl}m_jn_km_l)' = c'_{ijkl}m'_jn'_km'_l$$

= $c_{ijkl}(m_j)(-n_k)(m_l) = -c_{ijkl}m_jn_km_l.$ (4.5)

From (4.2)-(4.5), we can easily see that each of the vectors $U_{ij}n_j = c_{ijkk}n_j, V_{ij}n_j = c_{ikjk}n_j, W_{ik}(\mathbf{n})n_k = c_{ijkl}n_jn_kn_l$ and $W_{ik}(\mathbf{m})n_k = c_{ijkl}m_jn_km_l$ reverses its direction hence each of these vectors must be parallel to n_i , which implies that \mathbf{n} is an eigenvector of each of the tensors $\mathbf{U} = U_{ij} = c_{ijkk}, \ \mathbf{V} = V_{ij} = c_{ikjk}, \ W(\mathbf{n}) = W_{ik}(\mathbf{n}) = c_{ijkl}n_jn_l$ and $W(\mathbf{m}) = W_{ik}(\mathbf{m}) = c_{ijkl}m_jm_l$.

4.1.2 Axis of symmetry

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 vectors $U_{ij}p_j = c_{ijkk}p_j$, $V_{ij}p_j = c_{ikjk}p_j$, and $c_{ijkl}p_jp_kp_l$. These vectors will, respectively, transform as follows

$$(U_{ij}p_j)' = (c_{ijkk}p_j)' = c'_{ijkk}p'_j = c_{ijkk}p_j,$$
(4.6)

$$(V_{ij}n_j)' = (c_{ikjk}p_j)' = c'_{ikjk}p'_j = c_{ikjk}p_j, \qquad (4.7)$$

$$(c_{ijkl}p_{j}p_{k}p_{l})' = c'_{ijkl}p'_{j}p'_{k}p'_{l} = c_{ijkl}p_{j}p_{k}p_{l}.$$
(4.8)

From(4.6)-(4.8), it is clear that each of the vectors $U_{ij}p_j = c_{ijkk}p_j, V_{ij}p_j = c_{ikjk}p_j$, and $c_{ijkl}p_jp_kp_l$ are parallel to p_i leading to the result that \mathbf{p} is an eigenvector of each of the tensors $\mathbf{U} = U_{ij} = c_{ijkk}, \mathbf{V} = V_{ij} = c_{ikjk}, W_{il}(\mathbf{p}) = c_{ijkl}p_jp_k$ and $W_{ik}(\mathbf{p}) = c_{ijkl}p_jp_l$.

4.1.3 Necessary and sufficient conditions for an A_n -axis, $n \ge 3$.

If a tensor **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 [46]

$$(\mathbf{A}) = \begin{pmatrix} a_{11} & a_{12} & 0\\ -a_{12} & a_{11} & 0\\ 0 & 0 & a_{33} \end{pmatrix}.$$
 (4.9)

Thus any tensor of rank 2 associated with the elasticity tensor will have the above representation. The following Theorem uses this fact to characterize an axis of symmetry of a tensor 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 [31] that if \mathbf{p} is an axis of symmetry A_n , $n \ge 3$, it must be an eigenvector of both \mathbf{U} and \mathbf{V} belonging, in each case, to a nondegenerate eigenvalue.

Theorem 4.1. A set of necessary conditions for a unit vector \mathbf{p} to be an n-fold axis of symmetry, $A_n, n \ge 3$, is the following.

- (i) **p** is a common eigenvector of **U** and **V**, belonging to a nondegenerate eigenvalue.
- (ii) With coordinate axes chosen so that x₃-axis is along p, matrices representing the tensors U = c_{iikl}, V = c_{ijkj}, W₁(p) = c_{ijkl}p_kp_l and W₂(p) = c_{ijkl}p_jp_l are of the form (4.9).

Proof. Proof of the first condition being necessary is contained in the observations following (4.2)-(4.5). Since each of the four second rank tensors $\mathbf{U} = c_{iikl}, \mathbf{V} = c_{ijkj}, \mathbf{W}_1(\mathbf{p}) = c_{ijkl}p_kp_l$ and $\mathbf{W}_2(\mathbf{p}) = c_{ijkl}p_jp_l$, is invariant with respect to a transformation associated with a three fold, four fold or a six fold axis of symmetry, the matrix representation must be of the form (4.9). Note that, if we compare a symmetric matrix, $M = (m_{ij})$, with (4.9), 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 (see \mathbf{W}_3 in Theorem 4.7).

The conditions given above are necessary but not sufficient for the existence of an A_n axis, $n \ge 3$, to be an axis of symmetry. In order to find necessary and sufficient conditions,

- (a) $c_{16} = 0$, $c_{66} = \frac{c_{11} c_{12}}{2}$,
- (b) **p** is an eigenvector of $c_{ijkl}m_jm_l$, where **m** is a unit vector perpendicular to **p**.

Now we are able to formulate necessary and sufficient conditions for the existence of an A_n axis, for each case of n = 3, 4 and 6.

Theorem 4.2. Necessary and sufficient conditions for a unit vector \mathbf{p} to be a 3-fold axis of symmetry are conditions (i), (ii) of Theorem 4.1 and condition (a).

Proof. We choose x_3 -axis along **p** and consider the matrix representation of the tensor $c_{ijkl}p_kp_l = c_{ij33}$. Its matrix representation, in the two index notation, is

$$\left(\begin{array}{cccc} c_{13} & c_{36} & c_{35} \\ c_{36} & c_{23} & c_{34} \\ c_{35} & c_{34} & c_{33} \end{array}\right)$$

A comparison with (4.9) gives

$$c_{34} = c_{35} = c_{36} = 0, \ c_{13} = c_{23}. \tag{4.10}$$

Matrix representation of the tensor $c_{ijkl}p_jp_l = c_{i3k3}$ is

$$\left(\begin{array}{cccc} c_{55} & c_{45} & c_{35} \\ c_{45} & c_{44} & c_{34} \\ c_{35} & c_{34} & c_{33} \end{array}\right),$$

which leads to

$$c_{45} = 0, \ c_{44} = c_{55}. \tag{4.11}$$

The tensor c_{ijkj} has the representation

$$\left(\begin{array}{cccc} c_{11} + c_{66} + c_{55} & c_{16} + c_{26} + c_{45} & c_{15} + c_{46} + c_{35} \\ c_{16} + c_{26} + c_{45} & c_{66} + c_{22} + c_{44} & c_{56} + c_{24} + c_{34} \\ c_{15} + c_{46} + c_{35} & c_{56} + c_{24} + c_{34} & c_{55} + c_{44} + c_{33} \end{array}\right)$$

Comparison with (4.9) and use of (4.10) and (4.11) leads to

$$c_{16} + c_{26} = 0, \ c_{15} + c_{46} = 0, \ c_{24} + c_{56} = 0, \ c_{11} = c_{22}.$$
 (4.12)

Similarly, the tensor c_{iikl} has the representation

$$\begin{pmatrix} c_{11} + c_{12} + c_{13} & c_{16} + c_{26} + c_{36} & c_{15} + c_{25} + c_{35} \\ c_{16} + c_{26} + c_{36} & c_{12} + c_{22} + c_{23} & c_{14} + c_{24} + c_{34} \\ c_{15} + c_{25} + c_{35} & c_{14} + c_{24} + c_{34} & c_{13} + c_{23} + c_{33} \end{pmatrix}$$

Comparison with (4.9) and use of (4.10) and (4.11) leads to

$$c_{15} + c_{25} = 0, \ c_{14} + c_{24} = 0. \tag{4.13}$$

The 6×6 matrix representation of the elasticity tensor, with the use of (4.10)-(4.13), becomes

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

$$(4.14)$$

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

$$\left(\begin{array}{cccccccccccc} c_{11} & c_{12} & c_{13} & c_{14} & c_{15} & 0 \\ c_{12} & c_{11} & c_{13} & -c_{14} & -c_{15} & 0 \\ c_{13} & c_{13} & c_{33} & 0 & 0 & 0 \\ c_{14} & -c_{14} & 0 & c_{44} & 0 & -c_{15} \\ c_{15} & -c_{15} & 0 & 0 & c_{44} & c_{14} \\ 0 & 0 & 0 & -c_{15} & c_{14} & \frac{c_{11}-c_{12}}{2} \end{array}\right),$$

which shows the material possesses trigonal symmetry. This proves the Theorem. $\hfill\square$

Theorem 4.3. Necessary and sufficient conditions for a unit vector \mathbf{p} to be a 4-fold axis of symmetry are conditions (i), (ii) of Theorem 4.1 and condition (b).

Proof. Let us choose x_1 axis along \mathbf{m} , that is $\mathbf{m} = (1, 0, 0)^T$. The tensor $c_{ijkl}m_jm_l$ becomes c_{i1k1} , which has the matrix representation

$$\left(\begin{array}{cccc} c_{11} & c_{16} & c_{15} \\ c_{61} & c_{66} & c_{65} \\ c_{51} & c_{56} & c_{55} \end{array}\right)$$

Since $\mathbf{p} = (0, 0, 1)^T$ is an eigenvector of the above matrix, we can write

$$\begin{pmatrix} c_{11} & c_{16} & c_{15} \\ c_{61} & c_{66} & c_{65} \\ c_{51} & c_{56} & c_{55} \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = \lambda \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$
$$\begin{pmatrix} c_{15} \\ c_{65} \\ c_{55} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \lambda \end{pmatrix}$$
e corresponding to the eigenvector $\mathbf{p} = \mathbf{p}$

or

where λ is an eigenvalue corresponding to the eigenvector $\mathbf{p} = (0, 0, 1)^T$. We must have $c_{15} = c_{65} = 0$. But $c_{65} = c_{56} = c_{14}$. Therefore we have $c_{14} = c_{15} = 0$. The matrix (4.14) becomes

$$\left(\begin{array}{ccccccccccc} c_{11} & c_{12} & c_{13} & 0 & 0 & c_{16} \\ c_{12} & c_{11} & c_{13} & 0 & 0 & -c_{16} \\ c_{13} & c_{13} & c_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{44} & 0 \\ c_{16} & -c_{16} & 0 & 0 & 0 & c_{66} \end{array}\right)$$

,

which is the matrix representation of the elasticity tensor with an A_4 axis of symmetry [46]. This proves the Theorem.

Theorem 4.4. Necessary and sufficient conditions for a unit vector \mathbf{p} to be a 6-fold axis of symmetry are conditions (i), (ii) of Theorem 4.1 and conditions (a) and (b)

Proof. To prove this Theorem, we follow on the same lines as those for the proof of Theo-

rems 4.2 and 4.3. Additionally, if both (a) and (b) hold, the matrix (4.14) will become

$$\left(\begin{array}{ccccccccccc} c_{11} & c_{12} & c_{13} & 0 & 0 & 0 \\ c_{12} & c_{11} & c_{13} & 0 & 0 & 0 \\ c_{13} & c_{13} & c_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{c_{11}-c_{12}}{2} \end{array}\right),$$

which characterizes hexagonal symmetry. This proves Theorem 4.4.

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

$$\mathbf{R} = \begin{pmatrix} \cos \beta & 0 & -\sin \beta \\ 0 & 1 & 0 \\ \sin \beta & 0 & \cos \beta \end{pmatrix} \begin{pmatrix} \cos \alpha & \sin \alpha & 0 \\ -\sin \alpha & \cos \alpha & 0 \\ 0 & 0 & 1 \end{pmatrix}$$
$$= \begin{pmatrix} \cos \alpha \cos \beta & \sin \alpha \cos \beta & -\sin \beta \\ -\sin \alpha & \cos \alpha & 0 \\ \cos \alpha \sin \beta & \sin \alpha \sin \beta & \cos \beta \end{pmatrix}$$
(4.15)

is such that

$$\mathbf{Rq} = \begin{pmatrix} \cos\alpha\cos\beta & \sin\alpha\cos\beta & -\sin\beta \\ -\sin\alpha & \cos\alpha & 0 \\ \cos\alpha\sin\beta & \sin\alpha\sin\beta & \cos\beta \end{pmatrix} \begin{pmatrix} \cos\alpha\sin\beta \\ \sin\alpha\sin\beta \\ \cos\beta \end{pmatrix}$$
$$= \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}.$$

Thus **R** orients an arbitrary vector specified by its Euler angles α and β along x_3 -axis.

4.2 Plane of symmetry of a piezoelectric material

The argument leading to and following (4.2)-(4.5) will now be applied to the piezoelectric tensor **e** to find necessary and sufficient conditions for the existence of a plane of symmetry.

Theorem 4.5. 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 $\mathbf{v}_1 = e_{kjj}$, $\mathbf{v}_2 = e_{jjk}$, $\mathbf{v}_3(\mathbf{n}) = e_{ijk}n_in_j$,
- (a) it is parallel to each of the vectors $\mathbf{w}_1(\mathbf{n}, \mathbf{m}) = e_{ijk}n_im_j$, $\mathbf{w}_2(\mathbf{n}, \mathbf{m}) = e_{ijk}m_in_j$, $\mathbf{w}_3(\mathbf{n}, \mathbf{m}) = e_{kij}m_in_j$.

Proof. First suppose a plane of symmetry exists with normal \mathbf{n} . The vectors $\mathbf{v}_1 = e_{kjj}$, $\mathbf{v}_2 = e_{jjk}$, $\mathbf{v}_3(\mathbf{n}) = e_{ijk}n_in_j$ can be expressed as $\mathbf{v}_1 = \delta_{ij}e_{kij}$, $\mathbf{v}_2 = \delta_{ij}e_{ijk}$ and $\mathbf{v}_3 = e_{ijk}n_in_j$, respectively. Under the transformation associated with the plane, mentioned above, these vectors transform as

$$\mathbf{v}_1' = (\delta_{ij} e_{kij})' = \delta_{ij} e_{kij} = e_{kjj} = \mathbf{v}_1,$$
$$\mathbf{v}_2' = (\delta_{ij} e_{ijk})' = \delta_{ij} e_{ijk} = e_{jjk} = \mathbf{v}_2$$

and

$$\mathbf{v}_3' = (e_{ijk}n_in_j)' = e_{ijk}(-n_i)(-n_j) = e_{ijk}n_in_j = \mathbf{v}_3.$$

Thus each of the vectors \mathbf{v}_1 , \mathbf{v}_2 and \mathbf{v}_3 transforms into itself hence each of these vectors must be orthogonal to \mathbf{n} .

Next consider the transformations of $\mathbf{w}_1(\mathbf{n}, \mathbf{m}), \mathbf{w}_2(\mathbf{n}, \mathbf{m})$ and $\mathbf{w}_3(\mathbf{n}, \mathbf{m})$. We have

$$\mathbf{w}_{1}(\mathbf{n}, \mathbf{m})' = (e_{ijk}n_{i}m_{j})' = e_{ijk}(-n_{i})m_{j} = -e_{ijk}n_{i}m_{j},$$
$$\mathbf{w}_{2}(\mathbf{n}, \mathbf{m})' = (e_{ijk}m_{i}n_{j})' = e_{ijk}m_{i}(-n_{j}) = -e_{ijk}m_{i}n_{j}$$

and

$$\mathbf{w}_3(\mathbf{n},\mathbf{m})' = (e_{kij}m_in_j)' = e_{kij}m_i(-n_j) = -e_{kij}m_in_j$$

Thus $\mathbf{w}_1(\mathbf{n}, \mathbf{m})' = -\mathbf{w}_1(\mathbf{n}, \mathbf{m}), \mathbf{w}_2(\mathbf{n}, \mathbf{m})' = -\mathbf{w}_2(\mathbf{n}, \mathbf{m})$ and $\mathbf{w}_3(\mathbf{n}, \mathbf{m})' = -\mathbf{w}_3(\mathbf{n}, \mathbf{m})$ leading to the conclusion that each of the vectors $\mathbf{w}_1(\mathbf{n}, \mathbf{m}), \mathbf{w}_2(\mathbf{n}, \mathbf{m})$ and $\mathbf{w}_3(\mathbf{n}, \mathbf{m})$ must be parallel to \mathbf{n} .

To show that the conditions (a) and (b) of this theorem are sufficient, choose coordinate axes so that x_1 and x_3 axes are respectively aligned with **m** and **n** i.e. $\mathbf{m} = (1, 0, 0)^T$ and $\mathbf{n} = (0, 0, 1)^T$. Vectors $\mathbf{v}_1, \mathbf{v}_2$ and \mathbf{v}_3 , in components form, can be written as

$$\mathbf{v}_1 = (e_{11} + e_{12} + e_{13}, e_{21} + e_{22} + e_{23}, e_{31} + e_{32} + e_{33})^T,$$

$$\mathbf{v}_2 = (e_{11} + e_{26} + e_{35}, e_{16} + e_{22} + e_{34}, e_{15} + e_{24} + e_{33})^T,$$

$$\mathbf{v}_3 = (e_{31}, e_{32}, e_{33})^T.$$

The condition that \mathbf{n} be orthogonal to each of these vectors, leads to the following

$$e_{31} + e_{32} + e_{33} = 0,$$

 $e_{15} + e_{24} + e_{33} = 0,$
 $e_{33} = 0.$ (4.16)

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, therefore

$$\mathbf{n} \times \mathbf{w}_1(\mathbf{n}, \mathbf{m}) = (-e_{36}, e_{31}, 0)^T = (0, 0, 0),$$

$$\mathbf{n} \times \mathbf{w}_2(\mathbf{n}, \mathbf{m}) = (-e_{14}, e_{15}, 0)^T = (0, 0, 0),$$

$$\mathbf{n} \times \mathbf{w}_3(\mathbf{n}, \mathbf{m}) = (-e_{25}, e_{15}, 0)^T = (0, 0, 0),$$

imply that

$$e_{31} = e_{36} = e_{14} = e_{15} = e_{25} = 0. (4.17)$$

Equations (4.16) and (4.17) together imply

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

which reduces the matrix (2.70) to the form

$$\mathbf{e} = \left(\begin{array}{cccccc} e_{11} & e_{12} & e_{13} & 0 & 0 & e_{16} \\ e_{21} & e_{22} & e_{23} & 0 & 0 & e_{26} \\ 0 & 0 & 0 & e_{34} & e_{35} & 0 \end{array} \right),$$

so that the tensor \mathbf{e} has x_3 -axis as a normal to a plane of symmetry [46].

Example 1. Consider the following 3×6 matrix representing a piezoelectric tensor **d**.

$$\mathbf{d} = \begin{pmatrix} 4.7754 & -1.6177 & -2.6007 & -1.9427 & -0.13572 & -4.2248 \\ -1.7186 & 0.34562 & -0.49744 & 5.3860 & 3.4468 & 0.75776 \\ -0.10442 & -0.77998 & 1.1023 & -7.7468 & -3.0673 & -0.60562 \end{pmatrix}$$
(4.18)

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 $\alpha > 3$ [46].

We wish to determine wether or not a plane of symmetry exists. Vectors \mathbf{v}_1 and \mathbf{v}_2 can be readily obtained from (4.18) as

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

$$\mathbf{n} = \frac{\mathbf{v}_1 \times \mathbf{v}_2}{|\mathbf{v}_1 \times \mathbf{v}_2|} = (-.830497, -0.186178, 0.524988)^T.$$
(4.19)

We can take \mathbf{m} a unit vector along \mathbf{v}_1 ,

$$\mathbf{m} = \frac{\mathbf{v}_1}{|\mathbf{v}_1|} = (0.28366, -0.952485, 0.11095)^T.$$
(4.20)

We use (4.19) and compute the vector \mathbf{v}_3 as

$$\mathbf{v}_3 = (2.22809, -2.33557, 2.69643)^T,$$

which is orthogonal to **n**, because

$$\mathbf{n}.\mathbf{v}_3=0.$$

Similarly, by using (4.20) 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 **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

 $\mathbf{n} = (\cos \alpha \sin \beta, \sin \alpha \sin \beta, \cos \beta)^T = (-0.8305, -0.186176, 0.524984)^T$. Application of the transformation (4.15) to \mathbf{n} transforms it to $(0, 0, 1)^T$. That is

$$\mathbf{Rn} = \begin{pmatrix} -0.51227 & -0.114837 & -0.851112\\ 0.218744 & -0.975782 & 0\\ -0.8305 & -0.186176 & 0.524984 \end{pmatrix} \begin{pmatrix} -0.8305 \\ -0.186176 \\ 0.524984 \end{pmatrix}$$
$$= \begin{pmatrix} 0\\ 0\\ 1 \end{pmatrix}.$$

Same transformation applied to the tensor represented by (4.18) 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.

$$\mathbf{d}' = \left(\begin{array}{cccccccc} 1.60894 & 0.72657 & -2.59149 & 0 & 0 & 3.70196 \\ -1.48785 & -0.17272 & 3.60752 & 0 & 0 & -2.82030 \\ 0 & 0 & 0 & 2.76639 & -3.16813 & 0 \end{array} \right),$$

With coordinate axes so that x_2 -axis is along **n**, the tensor (4.18) transforms to

$$\mathbf{d}'' = \left(\begin{array}{ccccccccc} 1.4 & 3.8 & -4.2 & 0 & -7.2 & 0 \\ 0 & 0 & 0 & -2.6 & 0 & 8 \\ -0.22 & -2.3 & 0.83 & 0 & 2.2 & 0 \end{array}\right)$$

which is the tensor representing the YCOB crystal reported in [51].

4.3 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 $A_n, n \ge 3$ will be given in Theorems 4.7 and 4.8.

Theorem 4.6. 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 $\mathbf{v}_1 = e_{ijj}$, $\mathbf{v}_2 = e_{jjk}$, $\mathbf{v}_3(\mathbf{p}) = e_{ijk}p_ip_j$, $\mathbf{v}_4(\mathbf{p}) = e_{ijk}p_jp_k$, $\mathbf{v}_5(\mathbf{m}) = e_{ijk}m_im_j$, $\mathbf{v}_6(\mathbf{m}) = e_{ijk}m_jm_k$.

Proof. 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, (see [31]). Unlike the transformation defined by (2.28), used in the proof of Theorem 4.5, this transformation leaves every vector parallel to \mathbf{p} unchanged but reverses the direction of any vector orthogonal to \mathbf{p} . That is, $\mathbf{Q}\mathbf{p} = \mathbf{p}$ and $\mathbf{Q}\mathbf{m} = -\mathbf{m}$, where $\mathbf{m} \perp \mathbf{p}$. The vectors $\mathbf{v}_1 = e_{ijj}$, $\mathbf{v}_2 = e_{jjk}$ can be expressed as $\mathbf{v}_1 = \delta_{jk}e_{ijk}$, $\mathbf{v}_2 = \delta_{ij}e_{ijk}$, respectively. Under the transformation associated with rotation about an axis \mathbf{p} , mentioned above, these vectors transform as

$$\mathbf{v}_1' = (\delta_{jk} e_{ijk})' = \delta_{jk} e_{ijk} = e_{ijj} = \mathbf{v}_1,$$
$$\mathbf{v}_2' = (\delta_{ij} e_{ijk})' = \delta_{ij} e_{ijk} = e_{jjk} = \mathbf{v}_2,$$

similarly

$$\mathbf{v}_{3}'(\mathbf{p}) = (e_{ijk}p_{i}p_{j})' = e'_{ijk}p'_{i}p'_{j} = e_{ijk}p_{i}p_{j} = \mathbf{v}_{3}(\mathbf{p}),$$
$$\mathbf{v}_{4}'(\mathbf{p}) = (e_{ijk}p_{j}p_{k})' = e'_{ijk}p'_{j}p'_{k} = e_{ijk}p_{j}p_{k} = \mathbf{v}_{4}(\mathbf{p}),$$
$$\mathbf{v}_{5}'(\mathbf{m}) = (e_{ijk}m_{i}m_{j})' = e_{ijk}(-m_{i})(-m_{j}) = e_{ijk}m_{i}m_{j} = \mathbf{v}_{5}(\mathbf{m})$$

and

$$\mathbf{v}_6'(\mathbf{m}) = (e_{ijk}m_jm_k)' = e_{ijk}(-m_j)(-m_k) = e_{ijk}m_jm_k = \mathbf{v}_6(\mathbf{m}).$$

Thus each of the vectors \mathbf{v}_1 , \mathbf{v}_2 , $\mathbf{v}_3(\mathbf{p})$, $\mathbf{v}_4(\mathbf{p})$, $\mathbf{v}_5(\mathbf{m})$ and $\mathbf{v}_6(\mathbf{m})$ transforms into itself hence each of these vectors must be parallel to \mathbf{p} .

To show that the given condition is sufficient, choose coordinate axes so that x_1 and x_3 axes are respectively aligned with **m** and **p** i.e. $\mathbf{m} = (1, 0, 0)^T$ and $\mathbf{p} = (0, 0, 1)^T$. Vectors $\mathbf{v}_1, \ \mathbf{v}_2, \ \mathbf{v}_3(\mathbf{p}), \ \mathbf{v}_4(\mathbf{p}), \ \mathbf{v}_5(\mathbf{m}) \text{ and } \mathbf{v}_6(\mathbf{m}), \text{ in components form, can be written as}$

$$\begin{aligned} \mathbf{v}_1 &= (e_{11} + e_{12} + e_{13}, e_{21} + e_{22} + e_{23}, e_{31} + e_{32} + e_{33})^T, \\ \mathbf{v}_2 &= (e_{11} + e_{26} + e_{35}, e_{16} + e_{22} + e_{34}, e_{15} + e_{24} + e_{33})^T, \\ \mathbf{v}_3 &= (e_{35}, e_{34}, e_{33})^T, \\ \mathbf{v}_4 &= (e_{13}, e_{23}, e_{33})^T, \\ \mathbf{v}_5 &= (e_{11}, e_{16}, e_{15})^T \\ \mathbf{v}_6 &= (e_{11}, e_{21}, e_{31})^T, \end{aligned}$$

respectively. The condition that \mathbf{p} be parallel to each of these vectors, leads to the following

$$\mathbf{p} \times \mathbf{v}_{1} = (-e_{21} - e_{22} - e_{23}, e_{11} + e_{12} + e_{13}, 0)^{T} = (0, 0, 0),$$

$$\mathbf{p} \times \mathbf{v}_{2} = (-e_{16} - e_{22} - e_{34}, e_{11} + e_{26} + e_{35}, 0)^{T} = (0, 0, 0),$$

$$\mathbf{p} \times \mathbf{v}_{3}(\mathbf{p}) = (-e_{34}, e_{35}, 0)^{T} = (0, 0, 0),$$

$$\mathbf{p} \times \mathbf{v}_{4}(\mathbf{p}) = (-e_{23}, e_{13}, 0)^{T} = (0, 0, 0),$$

$$\mathbf{p} \times \mathbf{v}_{5}(\mathbf{m}) = (-e_{16}, e_{11}, 0)^{T} = (0, 0, 0),$$

$$\mathbf{p} \times \mathbf{v}_{6}(\mathbf{m}) = (-e_{21}, e_{11}, 0)^{T} = (0, 0, 0).$$

That is

$$e_{21} + e_{22} + e_{23} = 0,$$

$$e_{11} + e_{12} + e_{13} = 0,$$

$$e_{16} + e_{22} + e_{34} = 0,$$

$$e_{11} + e_{26} + e_{35} = 0$$
(4.21)

and

$$e_{11} = e_{13} = e_{16} = e_{21} = e_{23} = e_{34} = e_{35} = 0.$$

$$(4.22)$$

Equations (4.21) and (4.22) together imply that

$$e_{11} = e_{12} = e_{13} = e_{16} = e_{21} = e_{22} = e_{23} = e_{26} = e_{34} = e_{35} = 0,$$

which reduces the matrix (2.70) to the form

$$\mathbf{e} = \left(\begin{array}{cccccc} 0 & 0 & 0 & e_{14} & e_{15} & 0 \\ 0 & 0 & 0 & e_{24} & e_{25} & 0 \\ e_{31} & e_{32} & e_{33} & 0 & 0 & e_{36} \end{array}\right),$$

so that the tensor **e** has x_3 -axis as a 2-fold axis of symmetry of a piezoelectric material [46].

Example 2. Consider the following 3×6 matrix representation of the piezoelectric tensor **e** corresponding to a hypothetical material.

$$\mathbf{e} = \begin{pmatrix} -0.756897 & 1.55523 & -1.59723 & 0.0815332 & -0.299296 & 0.138140 \\ 1.52488 & -0.699927 & -1.65214 & 0.296613 & -0.0961851 & 0.222583 \\ -1.79313 & 1.78259 & 0.007407 & 1.80617 & 1.73614 & -0.068369 \end{pmatrix},$$
(4.23)

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

We wish to determine wether or not an axis of symmetry exists. Vectors \mathbf{v}_1 and \mathbf{v}_2 can be obtained from (4.23) 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

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

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 α and β pertaining to \mathbf{p} are respectively 0.802793 and 1.56807 and the transformation matrix (4.15) becomes

$$\mathbf{R} = \begin{pmatrix} 0.0018970 & 0.0019642 & -0.999996 \\ -0.719299 & 0.694701 & 0 \\ 0.694698 & 0.719296 & 0.002731 \end{pmatrix}.$$
 (4.24)

The above transformation aligns \mathbf{p} along x_3 -axis, that is

$$\mathbf{Rp} = \begin{pmatrix} 0.0018970 & 0.0019642 & -0.999996 \\ -0.719299 & 0.694701 & 0 \\ 0.694698 & 0.719296 & 0.002731 \end{pmatrix} \begin{pmatrix} 0.694698 \\ 0.719296 \\ 0.002731 \end{pmatrix}$$
$$= \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix},$$

and, with respect to the new coordinate axes, the piezoelectric tensor has the following matrix representation

$$\left(\begin{array}{ccccccc} 0 & 0 & 0 & -1.78917 & 2.5053 & 0 \\ 0 & 0 & 0 & -1.6053 & -0.20917 & 0 \\ -2.29798 & 0.317977 & 0.83 & 0 & 0 & -0.386904 \end{array}\right),$$

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 4.2-4.4 for the elasticity tensor.

Theorem 4.7. 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.

- (i) **p** is parallel to $\mathbf{v}_1 = e_{ijj}$ as well as $\mathbf{v}_2 = e_{jji}$.
- (ii) With coordinate axes chosen so that x₃-axis is along p, the matrices representing second rank tensors W₃ = e_{ijk}p_k and W₄ = e_{ijk}p_i are of the form (4.9).

Proof. Suppose an axis of symmetry exists. The vectors $\mathbf{v}_1 = e_{ijj}$ and $\mathbf{v}_2 = e_{jji}$ can be expressed as $\mathbf{v}_1 = \delta_{jk}e_{ijk}$ and $\mathbf{v}_2 = \delta_{jk}e_{jki}$, respectively. Under the transformation associated with rotation about an axis \mathbf{p} , that is, $\mathbf{Q} = -\mathbf{I} + 2 \mathbf{p} \otimes \mathbf{p}$ [31], these vectors transform as

$$\mathbf{v}_1' = (\delta_{jk} e_{ijk})' = \delta_{jk} e_{ijk} = e_{ijj} = \mathbf{v}_1,$$
$$\mathbf{v}_2' = (\delta_{jk} e_{jki})' = \delta_{jk} e_{jki} = e_{jji} = \mathbf{v}_2.$$

This shows that **p** is parallel to each of the vectors $\mathbf{v}_1 = e_{ijj}$ and $\mathbf{v}_2 = e_{jji}$. Similarly we have

$$\mathbf{W}_3' = (e_{ijk}p_k)' = e_{ijk}p_k = \mathbf{W}_3,$$
$$\mathbf{W}_4' = (e_{ijk}p_i)' = e_{ijk}p_i = \mathbf{W}_4.$$

Thus each of the $\mathbf{W}_3 = e_{ijk}p_k$ and $\mathbf{W}_4 = e_{ijk}p_i$ is invariant with respect to a transformation associated with a three fold axis of symmetry, the matrix representation must be of the form (4.9).

To show that the conditions are sufficient, we choose x_3 -axis parallel to \mathbf{p} i.e. $\mathbf{p} = (0, 0, 1)^T$. Vectors $\mathbf{v}_1, \mathbf{v}_2$, in components form, can be written as

$$\mathbf{v}_1 = (e_{11} + e_{12} + e_{13}, e_{21} + e_{22} + e_{23}, e_{31} + e_{32} + e_{33})^T,$$

$$\mathbf{v}_2 = (e_{11} + e_{26} + e_{35}, e_{16} + e_{22} + e_{34}, e_{15} + e_{24} + e_{33})^T,$$

respectively. Since \mathbf{p} is parallel to each of these vectors, therefore, we have

$$\mathbf{p} \times \mathbf{v}_1 = (-e_{21} - e_{22} - e_{23}, e_{11} + e_{12} + e_{13}, 0)^T = (0, 0, 0),$$

$$\mathbf{p} \times \mathbf{v}_2 = (-e_{16} - e_{22} - e_{34}, e_{11} + e_{26} + e_{35}, 0)^T = (0, 0, 0).$$

Or

$$e_{11} + e_{12} + e_{13} = 0,$$

$$e_{21} + e_{22} + e_{23} = 0,$$

$$e_{11} + e_{26} + e_{35} = 0,$$

$$e_{16} + e_{22} + e_{34} = 0.$$
(4.25)

Matrix representation of the tensor $\mathbf{W}_3 = e_{ijk}p_k = e_{ij3}$ is

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

A comparison with (4.9) gives

$$e_{15} = e_{24}, \ e_{14} = -e_{25}, \ e_{13} = e_{23} = e_{34} = e_{35} = 0.$$
 (4.26)

Similarly, the matrix representation of the tensor $\mathbf{W}_4 = e_{ijk}p_i = e_{3jk}$ is

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

which, on comparison with (4.9), leads to

$$e_{31} = e_{32}, \ e_{36} = -e_{36} = 0.$$
 (4.27)

Equations (4.25)-(4.27) imply that there are only six independent components of the tensor **e** and it will have the representation

$$\begin{pmatrix} e_{11} & -e_{11} & 0 & e_{14} & e_{15} & -e_{22} \\ -e_{22} & e_{22} & 0 & e_{15} & -e_{14} & -e_{11} \\ e_{31} & e_{31} & e_{33} & 0 & 0 & 0 \end{pmatrix},$$
(4.28)

which is the form of a tensor belonging to a trigonal material [46]. Thus the material has trigonal symmetry. $\hfill \Box$

Finally we have the following Theorem:

Theorem 4.8. Let \mathbf{m} and \mathbf{n} be mutually perpendicular unit vectors in the plane normal to \mathbf{p} . If, in addition to conditions (i) and (ii) of Theorem 4.7, the tensor e_{ijk} satisfies the condition

(iii) $e_{ijk}m_in_j + e_{ijk}m_jn_i = 0$,

then **p** is a 4-fold or a 6-fold axis of symmetry.

Proof. We can choose x_1 and x_2 axes respectively along **m** and **n**, that is $\mathbf{m} = (1, 0, 0)^T$ and $\mathbf{n} = (0, 1, 0)^T$. Condition (iii) of the Theorem becomes

$$e_{12k} + e_{21k} = 0. (4.29)$$

Equation (4.29) implies that

$$e_{16} = -e_{21}, e_{12} = -e_{26}, e_{14} = -e_{25}.$$

$$(4.30)$$

Use of the conditions given by (4.30) in (4.28) leads to

$$e_{11} = e_{22} = 0$$

and matrix in (4.28) becomes

$$\left(\begin{array}{cccccc} 0 & 0 & 0 & e_{14} & e_{15} & 0 \\ 0 & 0 & 0 & e_{15} & -e_{14} & 0 \\ e_{31} & e_{31} & e_{33} & 0 & 0 & 0 \end{array}\right),$$

which is precisely the matrix representation of the piezoelectric tensor possessing tetragonal or hexagonal symmetry [46]. Hence \mathbf{p} is a 4-fold or a 6-fold axis of symmetry.

4.3.1 Generalization to a tensor of arbitrary rank

The results developed in Sections 4.1 and 4.2 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, Özarslan and Mareci [52] 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. **n** is an eigenvector of each of the tensors of rank 2 obtained from **T** by letting any pair of indices free and contracting others in pairs. For example T_{ijkkll} , T_{klikjl} , are two such tensors.
- 2. **n** is an eigenvector of the tensor obtained by contracting any three pairs of indices of $T_{ijklmn}n_pn_q$ or any four pairs of $T_{ijklmn}n_pn_qn_rn_s$.

Similarly, if the same tensor \mathbf{T} describes some physical property of a material having an axis of symmetry about a unit vector \mathbf{p} , the following results will also hold.

- 3. **p** is an eigenvector of each of the tensors of rank 2 obtained from **T** by letting any pair of indices free and contracting others in pairs. For example T_{ijkkll}, T_{klikjl} are two such tensors.
- 4. **p** is an eigenvector of the tensor obtained by contracting any three pairs of indices of $T_{ijklmn}p_qp_r$ or any four pairs of $T_{ijklmn}p_qp_rp_sp_t$.

Chapter 5

Young's modulus in hexagonal materials

In this chapter we shall apply the representation derived for a hexagonal material in chapter 3 to find an expression for $E(\mathbf{n})$ and consider its optimum values.

Our motivation comes from Norris [35] who considered Poisson's ratio in cubic materials. He found evidence for Poisson's ratio less than -1 in a certain direction and greater than 2 in some other direction. Norris has expressed the Young's modulus in term of invariant quantities, i.e. in terms of eigenvalues. On the other hand, Cazzani and Rovati [53] (also see [54]) have expressed the young's modulus in terms of the elastic compliances and the parameters which are also dependent on these elastic constants. Ting [49] has also obtained the explicit expressions of Young's modulus for hexagonal materials in terms of elastic compliances and discussed its direction surfaces. We shall also give an alternate way for finding the extreme values of Young's modulus in hexagonal materials.

This chapter consists of two sections. The first section is about Young's modulus in cubic materials, we have discussed the problem considered by Norris [35] in detail and reformulated it in six dimensions by applying the representation derived for a cubic material in chapter 3 to find an expression for $E(\mathbf{n})$. In section two, Young's modulus in hexagonal materials is explained and the extreme values of Young's modulus are discussed. The results obtained in this section are illustrated by some examples of real materials.

5.1 Cubic materials

Norris used a result of Walpole [32] to express the compliance tensor s for a cubic material in the form

$$s = \frac{1}{3k}J + \frac{1}{2\mu_1}(I - D) + \frac{1}{2\mu_2}(D - J)$$
(5.1)

where

$$I_{ijkl} = \frac{1}{2} (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk})$$

$$J_{ijkl} = \frac{1}{3} \delta_{ij} \delta_{kl}$$

$$D_{ijkl} = \delta_{i1} \delta_{j1} \delta_{k1} \delta_{l1} + \delta_{i2} \delta_{j2} \delta_{k2} \delta_{l2} + \delta_{i3} \delta_{j3} \delta_{k3} \delta_{l3}.$$
(5.2)

The parameters k, μ_1, μ_2 are related to the Voigt notation for the stiffness tensor as follows

$$k = \frac{c_{11} + 2c_{12}}{3}$$

$$\mu_1 = c_{44}$$

$$\mu_2 = \frac{c_{11} - c_{12}}{2}$$
(5.3)

i.e. 3k, $2\mu_1$ and $2\mu_2$ are eigenvalues of the elasticity tensor in the Cowin-Mehrabadi formalism. Young's modulus in the direction specified by a unit vector $\mathbf{n} = (n_1, n_2, n_3)^T$ is defined by (2.80) or (2.81), that is as

$$E(\mathbf{n}) = \frac{1}{s_{ijkl}n_in_jn_kn_l}$$

or

$$\frac{1}{E(\mathbf{n})} = s_{ijkl} n_i n_j n_k n_l.$$

Norris [35] has simplified the formula in (2.85) as follows:

Let

$$n_2^2 n_3^2 + n_3^2 n_1^2 + n_1^2 n_2^2 = F(\mathbf{n}),$$
(5.4)

Substituting (5.3) and (5.4) into (2.85) and using $n_1^2 + n_2^2 + n_3^2 = 1$, we have

$$\frac{1}{E(\mathbf{n})} = s_{11} - 2s_{11}F(\mathbf{n}) + (\frac{1}{\mu_1} + 2s_{12})F(\mathbf{n})$$
$$= s_{11} - 2(s_{11} - s_{12})F(\mathbf{n}) + \frac{1}{\mu_1}F(\mathbf{n})$$
$$= s_{11} - \frac{1}{\mu_2}F(\mathbf{n}) + \frac{1}{\mu_1}F(\mathbf{n}).$$

The value of s_{11} in terms of k and μ_2 can be find as

$$s_{11} = \frac{1}{9k} + \frac{1}{3\mu_2}$$

Thus $\frac{1}{E(\mathbf{n})}$ has the following form

$$\frac{1}{E(\mathbf{n})} = \frac{1}{9k} + \frac{1}{3\mu_2} - \frac{1}{\mu_2}F(\mathbf{n}) + \frac{1}{\mu_1}F(\mathbf{n}),$$

$$= \frac{1}{9k} + \frac{1}{3\mu_2} - (\frac{1}{\mu_2} - \frac{1}{\mu_1})F(\mathbf{n}),$$
(5.5)

which is the result derived by Norris [35].

It is easy to show that

$$0 \leqslant F \leqslant \frac{1}{3} \tag{5.6}$$

A simple proof is as follows.

Let

$$f(n_1, n_2, n_3) = n_1^2 n_2^2 + n_2^2 n_3^2 + n_3^2 n_1^2 - \lambda (n_1^2 + n_2^2 + n_3^2)$$
(5.7)

where λ is a lagrange multiplier. Equating the derivatives of f with respect to n_1 , n_2 and n_3 to zero we find

$$2(n_2^2 + n_3^2) - 2n_1\lambda = 0$$

$$2(n_1^2 + n_3^2) - 2n_2\lambda = 0$$

$$2(n_1^2 + n_2^2) - 2n_3\lambda = 0$$
(5.8)

If $n_1 = 0$, $n_2 \neq 0$, $n_3 \neq 0$, then $\lambda = n_3^2 = n_2^2 = \frac{1}{2}$. Hence $F(\mathbf{n}) = \frac{1}{4}$. If two of n_1 , n_2 and n_3 vanish then $F(\mathbf{n}) = 0$. If none of them vanishes then

$$\lambda = n_2^2 + n_3^2 = n_1^2 + n_3^2 = n_1^2 + n_2^2$$

which implies $n_1^2 = n_2^2 = n_3^2 = \frac{1}{3}$ and $F(n) = \frac{1}{3}$. Thus $0 \leq F \leq \frac{1}{3}$. It shows that $F(\mathbf{n})$ attains its optimum value when it is aligned parallel to a body diagonal.

From (5.5) it is clear that, if $\frac{1}{\mu_1} \ge \frac{1}{\mu_2}$ then

$$\max \frac{1}{E} = \frac{1}{9k} + \frac{1}{3\mu_1},$$
$$\min \frac{1}{E} = \frac{1}{9k} + \frac{1}{3\mu_2}.$$

Also if $\frac{1}{\mu_1} \leqslant \frac{1}{\mu_2}$ then

$$\max \frac{1}{E} = \frac{1}{9k} + \frac{1}{3\mu_2},$$
$$\min \frac{1}{E} = \frac{1}{9k} + \frac{1}{3\mu_1}.$$

Cazzani and Rovati [53] have also obtained the above results but they have expressed $\frac{1}{E}$ in terms of components of the compliance tensor rather than the invariant expressions used above. Now we shall obtain (5.5) by using our representation of \hat{c} in chapter 3. In chapter 3, we have shown that the elasticity tensor may be represented as

$$\hat{c} = \lambda_1 F_1 + \lambda_2 F_2 + \lambda_4 F_3.$$

Hence the compliance tensor becomes

$$\hat{s} = \frac{1}{\lambda_1}F_1 + \frac{1}{\lambda_2}F_2 + \frac{1}{\lambda_4}F_3$$

where F_1 , F_2 and F_3 are given in chapter 3.

Now if $\mathbf{n} = (n_1, n_2, n_3)^T$ then $\hat{\mathbf{N}} = (n_1^2, n_2^2, n_3^2, \sqrt{2}n_2n_3, \sqrt{2}n_3n_1, \sqrt{2}n_1n_2)^T$. To calculate $s_{ijkl}n_in_jn_kn_l$, we simply need to find $\hat{\mathbf{N}}^T \hat{\mathbf{s}} \hat{\mathbf{N}}$. That is

$$\frac{1}{E(\mathbf{n})} = \hat{\mathbf{N}}^T \hat{\mathbf{s}} \hat{\mathbf{N}}.$$
(5.9)

Since

we find that

$$\hat{\mathbf{N}}^T F_1 \hat{\mathbf{N}} = \frac{1}{3} (n_1^2 + n_2^2 + n_3^2) = \frac{1}{3}$$

Also

thus

$$\hat{\mathbf{N}}^{T} F_{2} \hat{\mathbf{N}} = \frac{1}{3} (3n_{1}^{4} + 3n_{2}^{4} + 3n_{3}^{4} - n_{1}^{2} - n_{2}^{2} - n_{3}^{2})$$

$$= \frac{1}{3} (3[(n_{1}^{2} + n_{2}^{2} + n_{3}^{2})^{2} - 2n_{1}^{2}n_{2}^{2} - 2n_{2}^{2}n_{3}^{2} - 2n_{3}^{2}n_{1}^{2}] - 1)$$

$$= \frac{1}{3} (3[1 - 2F(\mathbf{n})] - 1)$$

$$= \frac{1}{3} (3 - 6F(\mathbf{n}) - 1)$$

$$= \frac{2}{3} - 2F(\mathbf{n}).$$

Finally

therefore

$$\hat{\mathbf{N}}^T F_3 \hat{\mathbf{N}} = 2(n_1^2 n_2^2 + n_2^2 n_3^2 + n_3^2 n_1^2)$$
$$= 2F(\mathbf{n}).$$

Hence (5.9) becomes

$$\frac{1}{E(\mathbf{n})} = \frac{1}{\lambda_1} \hat{\mathbf{N}}^T F_1 \hat{\mathbf{N}} + \frac{1}{\lambda_2} \hat{\mathbf{N}}^T F_2 \hat{\mathbf{N}} + \frac{1}{\lambda_4} \hat{\mathbf{N}}^T F_3 \hat{\mathbf{N}}$$
$$= \frac{1}{3\lambda_1} + \frac{2}{3\lambda_2} + 2(\frac{1}{\lambda_4} - \frac{1}{\lambda_2})F(\mathbf{n}).$$
(5.10)

This is identical to (5.5) if we identify $\lambda_1 = 3k$, $\lambda_2 = 2\mu_2$ and $\lambda_4 = 2\mu_1$. Thus our formulation gives the same results as those of Norris [35] and Cazzani and Rovati [53]. Next we shall use our results of chapter 3 to express Young's modulus in terms of eigenvalues of the elasticity tensor and an arbitrary parameter.

5.2 Transversely isotropic (hexagonal) materials

In chapter 3, we have shown that the elasticity tensor for transversely isotropic (hexagonal) materials may be represented as

$$\hat{c} = \lambda_1 E_1 + \lambda_2 E_2 + \lambda_3 (E_3 + E_4) + \lambda_5 (E_5 + E_6).$$
(5.11)

Hence the compliance tensor becomes

$$\hat{s} = \frac{1}{\lambda_1} E_1 + \frac{1}{\lambda_2} E_2 + \frac{1}{\lambda_3} (E_3 + E_4) + \frac{1}{\lambda_5} (E_5 + E_6)$$
(5.12)

where E_1 , E_2 , $E_3 + E_4$ and $E_5 + E_6$ are given in chapter 3.

The value of $\frac{1}{E(\mathbf{n})} = \hat{\mathbf{N}}^T \hat{\mathbf{s}} \hat{\mathbf{N}}$ can be calculated as follows:

so that

$$\hat{\mathbf{N}}^{T} E_{1} \hat{\mathbf{N}} = \frac{1}{2+a^{2}} [n_{1}^{2}(n_{1}^{2}+n_{2}^{2}+n_{3}^{2}a) + n_{2}^{2}(n_{1}^{2}+n_{2}^{2}+n_{3}^{2}a) + n_{3}^{2}a(n_{1}^{2}+n_{2}^{2}) + a^{2}n_{3}^{4}]$$

$$= \frac{1}{2+a^{2}} [n_{1}^{2}(n_{1}^{2}+n_{2}^{2}+n_{3}^{2}a) + n_{2}^{2}(n_{1}^{2}+n_{2}^{2}+n_{3}^{2}a) + n_{3}^{2}a(n_{1}^{2}+n_{2}^{2}+an_{3}^{2}]$$

$$= \frac{1}{2+a^{2}} (n_{1}^{2}+n_{2}^{2}+n_{3}^{2}a)^{2}$$

$$= \frac{1}{2+a^{2}} [1 + (a-1)n_{3}^{2}]^{2}.$$

Next we calculate

thus

$$\hat{\mathbf{N}}^{T} E_{2} \hat{\mathbf{N}} = \frac{1}{4 + 2a^{2}} [a^{2}n_{1}^{2}(n_{1}^{2} + n_{2}^{2}) - 2an_{1}^{2}n_{3}^{2} + a^{2}n_{2}^{2}(n_{1}^{2} + n_{2}^{2}) - 2an_{2}^{2}n_{3}^{2} - 2an_{3}^{2}(n_{1}^{2} + n_{2}^{2}) + 4n_{3}^{4}]$$

$$= \frac{1}{4 + 2a^{2}} [a(n_{1}^{2} + n_{2}^{2})(an_{1}^{2} + an_{2}^{2} - 2n_{3}^{2}) - 2n_{3}^{2}(an_{1}^{2} + an_{2}^{2} - 2n_{3}^{2})]$$

$$= \frac{1}{4 + 2a^{2}} [a(n_{1}^{2} + n_{2}^{2}) - 2n_{3}^{2}]^{2}$$

$$= \frac{1}{4 + 2a^{2}} [(a + 2)n_{3}^{2} - a]^{2}.$$

Similarly

and

Thus we have

$$\frac{1}{E(\mathbf{n})} = \mathbf{\hat{N}}^{T} \mathbf{\hat{s}} \mathbf{\hat{N}}$$

$$= \frac{1}{\lambda_{1}} \mathbf{\hat{N}}^{T} E_{1} \mathbf{\hat{N}} + \frac{1}{\lambda_{2}} \mathbf{\hat{N}}^{T} E_{2} \mathbf{\hat{N}} + \frac{1}{\lambda_{3}} \mathbf{\hat{N}}^{T} (E_{3} + E_{4}) \mathbf{\hat{N}} + \frac{1}{\lambda_{5}} \mathbf{\hat{N}}^{T} (E_{5} + E_{6}) \mathbf{\hat{N}}$$

$$= \frac{1}{\lambda_{1}} \frac{[1 + (a - 1)n_{3}^{2}]^{2}}{2 + a^{2}} + \frac{1}{2\lambda_{2}} \frac{[(a + 2)n_{3}^{2} - a]^{2}}{2 + a^{2}} + \frac{1}{2\lambda_{3}} (1 - n_{3}^{2})^{2} + \frac{2}{\lambda_{5}} n_{3}^{2} (1 - n_{3}^{2}).$$
(5.13)

We note that if $n_3 = 1$, the Young's modulus depends only on λ_1 and λ_2 . In this direction

$$\frac{1}{E(\mathbf{n})} = \frac{1}{\lambda_1} \frac{a^2}{2+a^2} + \frac{1}{\lambda_2} \frac{2}{2+a^2}$$
(5.14)

For a cubic material, $\frac{1}{E(\mathbf{n})}$, in a direction parallel to one of the coordinate axes, given by Eq. (5.10) becomes

$$\frac{1}{E(\mathbf{n})} = \frac{1}{3\lambda_1} + \frac{2}{3\lambda_2}.$$

We shall get the same result in the present case if we let a = 1 in (5.14). Thus there exists a transversely isotropic material closest to a cubic material in this sense.

Equation (5.13) is a function of n_3 only, that is $\frac{1}{E(n)} = \frac{1}{E(n_3)}$. For convenience, we let

$$\frac{1}{E(n_3)} = f(n_3). \tag{5.15}$$

To find the extremal direction, the derivative of $f(n_3)$ with respect to n_3 must be equal to zero. This gives

$$f'(n_3) = \frac{4n_3(a-1)[1+(a-1)n_3^2]}{\lambda_1(2+a^2)} + \frac{2n_3(a+2)[(a+2)n_3^2-a]^2}{\lambda_2(2+a^2)} - \frac{2n_3(1-n_3^2)}{\lambda_3} + \frac{4n_3(1-2n_3^2)}{\lambda_5} = 0$$

From this we find

$$n_3 = 0$$
 (5.16)

or

$$\left(\frac{1}{\lambda_3} - \frac{4}{\lambda_5} + \frac{2(a-1)^2}{\lambda_1(2+a^2)} + \frac{(a+2)^2}{\lambda_2(2+a^2)}\right)n_3^2 = \frac{1}{\lambda_3} - \frac{2}{\lambda_5} - \frac{2(a-1)}{\lambda_1(2+a^2)} + \frac{a(a+2)}{\lambda_2(2+a^2)}$$

which gives us

$$n_3 = \pm p$$
, say,

where,

$$p = \sqrt{\frac{\frac{1}{\lambda_3} - \frac{2}{\lambda_5} - \frac{2(a-1)}{\lambda_1(2+a^2)} + \frac{a(a+2)}{\lambda_2(2+a^2)}}{\frac{1}{\lambda_3} - \frac{4}{\lambda_5} + \frac{2(a-1)^2}{\lambda_1(2+a^2)} + \frac{(a+2)^2}{\lambda_2(2+a^2)}}}.$$
(5.17)

In order that n_3 be real we require the following pairs of inequalities

$$\frac{1}{\lambda_2} + \frac{1}{\lambda_3} - \frac{2}{\lambda_5} + \frac{2(a-1)}{2+a^2} \left(\frac{1}{\lambda_2} - \frac{1}{\lambda_1}\right) > 0$$
 (5.18a)

and

$$\frac{2}{\lambda_1} + \frac{1}{\lambda_2} + \frac{1}{\lambda_3} - \frac{4}{\lambda_5} + \frac{2(2a+1)}{2+a^2} \left(\frac{1}{\lambda_2} - \frac{1}{\lambda_1}\right) > 0$$
(5.18b)

or

$$\frac{1}{\lambda_2} + \frac{1}{\lambda_3} - \frac{2}{\lambda_5} + \frac{2(a-1)}{2+a^2} \left(\frac{1}{\lambda_2} - \frac{1}{\lambda_1}\right) < 0$$
 (5.19a)

and

$$\frac{2}{\lambda_1} + \frac{1}{\lambda_2} + \frac{1}{\lambda_3} - \frac{4}{\lambda_5} + \frac{2(2a+1)}{2+a^2} \left(\frac{1}{\lambda_2} - \frac{1}{\lambda_1}\right) < 0.$$
(5.19b)

On the other hand, if (5.18a,b) or (5.19a,b) are not satisfied, the Young's modulus will attains its extreme values in the symmetry plane. But if (5.18a,b) or (5.19a,b) are satisfied, then we find the extreme values of Young's modulus as follows:

The second derivative of $f(n_3)$ with respect to n_3 has the following expression

$$f''(n_3) = \frac{4(-1+a+3n_3^2-6an_3^2+3a^2n_3^2)}{\lambda_1(2+a^2)} + \frac{2(2+a)[6n_3^2+a(3n_3^2-1)]}{\lambda_2(2+a^2)} + \frac{4n_3^2-2(1-n_3^2)}{\lambda_3} + \frac{4(1-n_3^2)-20n_3^2}{\lambda_5}$$
(5.20)

Now we substitute the value of $n_3 = \pm p, 0$ into (5.20), respectively, we have

$$f''(\pm p) = -\frac{8(a-1)}{(2+a^2)\lambda_1} + \frac{4a(2+a)}{(2+a^2)\lambda_2} + \frac{4}{\lambda_3} - \frac{8}{\lambda_5}$$
$$= 4\left[\left(\frac{1}{\lambda_2} + \frac{1}{\lambda_3} - \frac{2}{\lambda_5}\right) + 2\frac{a-1}{2+a^2}\left(\frac{1}{\lambda_2} - \frac{1}{\lambda_1}\right)\right]$$
(5.21)

Note that the right hand side of (5.21) is identical, except for a factor of 4, to the left hand side of (5.18a).

$$f''(0) = \frac{4(a-1)}{(2+a^2)\lambda_1} + \frac{2a(2+a)}{(2+a^2)\lambda_2} - \frac{2}{\lambda_3} + \frac{4}{\lambda_5}$$

= $2\left[\left(\frac{2}{\lambda_5} - \frac{1}{\lambda_2} - \frac{1}{\lambda_3}\right) + 2\frac{a-1}{2+a^2}\left(\frac{1}{\lambda_1} - \frac{1}{\lambda_2}\right)\right]$
= $-2\left[\left(\frac{1}{\lambda_2} + \frac{1}{\lambda_3} - \frac{2}{\lambda_5}\right) + 2\frac{a-1}{2+a^2}\left(\frac{1}{\lambda_2} - \frac{1}{\lambda_1}\right)\right]$ (5.22)

We note that

$$f''(0) = -\frac{1}{2}f''(\pm p).$$

From the above equations, we conclude the following.

(i) If conditions (5.18) are satisfied then there is a minimum of $\frac{1}{E(\mathbf{n})}$ in the direction $n_3 = \pm p$ and a maximum when $n_3 = 0$ i.e. in the plane of isotropy.

- (ii) If conditions (5.19) are satisfied then there is a maximum of $\frac{1}{E(\mathbf{n})}$ in the direction $n_3 = \pm p$ and a minimum when $n_3 = 0$ i.e. in the plane of isotropy.
- (iii) When neither (5.18) nor (5.19) are satisfied, there is no maximum or minimum in any direction not lying in the plane of isotropy.

5.3 Applications to some real materials

Hexagonal materials, in Cowin-Mehrabadi formalism, are represented by the following 6×6 matrix

$$\hat{\mathbf{c}}_{\alpha\beta} = \begin{pmatrix} \hat{c}_{11} & \hat{c}_{12} & \hat{c}_{13} & 0 & 0 & 0 \\ \hat{c}_{12} & \hat{c}_{22} & \hat{c}_{13} & 0 & 0 & 0 \\ \hat{c}_{13} & \hat{c}_{13} & \hat{c}_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & 2\hat{c}_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & 2\hat{c}_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & \hat{c}_{11} - \hat{c}_{12} \end{pmatrix}$$
(5.23)

We want to apply the results of section 5.2 to some real materials.

Example 1.

Consider Beryllium (*Be*) as an example of the hexagonal materials, belong to the class 6/mmm for which the elastic stiffness constants are as reported in [46] as $c_{11} = 29.23$, $c_{12} = 2.67$, $c_{13} = 1.4$, $c_{33} = 33.64$ and $c_{44} = 16.25$. These constants are in units of $10^{10}N/m^2$. We wish to find the extreme values of Young's modulus for this data. The matrix in (5.23), in this case, becomes

$$\hat{\mathbf{c}}_{\alpha\beta} = \begin{pmatrix} 29.23 & 2.67 & 1.4 & 0 & 0 & 0 \\ 2.67 & 29.23 & 1.4 & 0 & 0 & 0 \\ 1.4 & 1.4 & 33.64 & 0 & 0 & 0 \\ 0 & 0 & 0 & 32.5 & 0 & 0 \\ 0 & 0 & 0 & 0 & 32.5 & 0 \\ 0 & 0 & 0 & 0 & 0 & 26.56 \end{pmatrix}.$$
(5.24)
The eigenvalues and the corresponding eigenvectors of this matrix are

$$\lambda_{1} = 34.9326, \ v_{1} = (0.386558, 0.386558, 0.837344, 0, 0, 0)^{T}$$
$$\lambda_{2} = 30.6074, \ v_{2} = (-0.592092, -0.592092, 0.546676, 0, 0, 0)^{T}$$
$$\lambda_{3} = \lambda_{4} = 26.56, \ v_{3} = (0, 0, 0, 0, 0, 1)^{T}, \ v_{4} = (0.707107, -0.707107, 0, 0, 0, 0)^{T}$$
$$\lambda_{5} = \lambda_{6} = 32.5, \ v_{5} = (0, 0, 0, 1, 0, 0)^{T} \ v_{6} = (0, 0, 0, 0, 1, 0)^{T}.$$
(5.25)

To find the value of the parameter a, we compare the first two eigenvectors in (5.25) to the corresponding eigenvectors of hexagonal materials obtained in (3.35) of chapter 3, that is

$$v_1 = \frac{1}{\sqrt{2+a^2}} (1, 1, a, 0, 0, 0)^T,$$

$$v_2 = \frac{1}{\sqrt{4+2a^2}} (a, a, -2, 0, 0, 0)^T.$$
(5.26)

As the first two eigenvectors in (5.25) are proportional to $(1, 1, 2.16615, 0, 0, 0)^T$ and $(2.16615, 2.16615, -2, 0, 0, 0)^T$, respectively, therefore a = 2.16615. Substituting the values of $\lambda_1, \lambda_2, \lambda_3, \lambda_5$ and a into the left hand sides of (5.18), we have

$$\frac{1}{\lambda_2} + \frac{1}{\lambda_3} - \frac{2}{\lambda_5} + \frac{2(a-1)}{2+a^2} \left(\frac{1}{\lambda_2} - \frac{1}{\lambda_1}\right) = 0.0101938 > 0$$

and

$$\frac{2}{\lambda_1} + \frac{1}{\lambda_2} + \frac{1}{\lambda_3} - \frac{4}{\lambda_5} + \frac{2(2a+1)}{2+a^2} \left(\frac{1}{\lambda_2} - \frac{1}{\lambda_1}\right) = 0.0109452 > 0.$$

That is conditions (5.18) are satisfied and the value of p is 0.965067, which is a real number. Thus we have $f''(\pm 0.965067) > 0$ and f''(0) < 0. Which means that there is a minimum of $\frac{1}{E(\mathbf{n})}$ in the direction $n_3 = \pm 0.965067$ and a maximum when $n_3 = 0$ i.e. in the plane of isotropy. As a result the Young's modulus $E(\mathbf{n})$ has a maximum at $n_3 = \pm 0.965067$ and a minimum at $n_3 = 0$. By using (5.13), the explicit values of maximum and minimum values of Young's modulus $E(\mathbf{n})$ can be found as follows:

$$\max E(\mathbf{n}) = E(\mathbf{n})|_{\text{at } n_3 = \pm p} = 33.5461$$
$$\min E(\mathbf{n}) = E(\mathbf{n})|_{\text{at } n_3 = 0} = 28.9379.$$

Example 2

Consider another example of Titanium (Ti) which is a hexagonal material of class 6/mmm. The elastic stiffness constants for Ti [46] are $c_{11} = 16.24$, $c_{12} = 9.20$, $c_{13} = 6.90$, $c_{33} = 18.07$ and $c_{44} = 4.67$. The matrix in (5.23), for this data, becomes

$$\hat{\mathbf{c}}_{\alpha\beta} = \begin{pmatrix} 16.24 & 9.20 & 6.90 & 0 & 0 & 0 \\ 9.20 & 16.24 & 1.4 & 0 & 0 & 0 \\ 6.90 & 6.90 & 18.07 & 0 & 0 & 0 \\ 0 & 0 & 0 & 9.34 & 0 & 0 \\ 0 & 0 & 0 & 0 & 9.34 & 0 \\ 0 & 0 & 0 & 0 & 0 & 7.04 \end{pmatrix}.$$
(5.27)

The eigenvalues and the corresponding eigenvectors of this matrix are

$$\lambda_{1} = 32.1857, \ v_{1} = (-0.581654, -0.581654, -0.568646, 0, 0, 0)^{T}$$

$$\lambda_{2} = 11.3243, \ v_{2} = (-0.402093, -0.402093, 0.822583, 0, 0, 0)^{T}$$

$$\lambda_{3} = \lambda_{4} = 7.04, \ v_{3} = (0, 0, 0, 0, 0, 1)^{T}, \ v_{4} = (0.707107, -0.707107, 0, 0, 0, 0)^{T}$$

$$\lambda_{5} = \lambda_{6} = 9.34, \ v_{5} = (0, 0, 0, 1, 0, 0)^{T}, \ v_{6} = (0, 0, 0, 0, 1, 0)^{T}.$$
(5.28)

As the first two eigenvectors in (5.28) are proportional to $(1, 1, 0.977636, 0, 0, 0)^T$ and $(0.977636, 0.977636, -2, 0, 0, 0)^T$ respectively. Therefore a = 0.977636. Substituting the values of $\lambda_1, \lambda_2, \lambda_3, \lambda_5$ and a into the left hand sides of (5.18), we have

$$\frac{1}{\lambda_2} + \frac{1}{\lambda_3} - \frac{2}{\lambda_5} + \frac{2(a-1)}{2+a^2} \left(\frac{1}{\lambda_2} - \frac{1}{\lambda_1}\right) = 0.0153521 > 0$$

and

$$\frac{2}{\lambda_1} + \frac{1}{\lambda_2} + \frac{1}{\lambda_3} - \frac{4}{\lambda_5} + \frac{2(2a+1)}{2+a^2} \left(\frac{1}{\lambda_2} - \frac{1}{\lambda_1}\right) = -0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.0213227 < 0.02127 < 0.02127 < 0.02127 < 0.02127 < 0.02127 < 0.02127 < 0.02127 < 0.02127 < 0.02127 < 0.02127 < 0$$

As neither (5.18) nor (5.19) are satisfied, therefore the real value of p does not exist. Thus for Titanium (Ti), there is no maximum or minimum of Young's modulus in any direction not lying in the plane of isotropy.

Also equation (5.22) gives

$$f''(0) = -0.0307044 < 0.$$

Therefore $\frac{1}{E(\mathbf{n})}|_{\text{at }n_3=0} = 0.958114$ is a maximum in any direction in the plane of symmetry. It has no maximum in any direction. Finally, we conclude that the minimum value of Young's modulus $E(\mathbf{n})$ in any direction of the plane of isotropy, i.e. $n_3 = 0$ is

$$\min E(\mathbf{n}) = E(\mathbf{n})|_{\text{at } n_3 = 0} = 10.4372$$

and the Young's modulus has no maximum in any direction.

Chapter 6

Summary

In this thesis we studied the symmetries of elasticity tensor and some problems concerning with this theory. Some results developed here are also extended to tensors of arbitrary rank that describe various physical quantities. Topics in this thesis provide an important tool for further study in material science, seismology, mathematical modeling and other fields of science which deal with these quantities. In this chapter we give the summary of this thesis which clearly shows that which results are obtained in this thesis and what is taken from other sources.

In the first two chapters, an overview of the literature and concerned research work is given in detail. The more important topics discussed here are commuting matrices (Theorem 2.1), Cowin-Mehrabadi formalism [11], Cowin-Mehrabadi Theorem [28] and its modified versions by many authors [21, 29–31] (Theorem 2.2-2.12), piezoelectricity and Young's modulus.

In chapter 3, we utilized the well-known results of linear algebra which play important role in enriching the theory of elasticity tensors. For this purpose we used Theorem 2.1 and Cowin-Mehrabadi formalism [11] in this chapter.

If a tensor is invariant under rotation about a fixed axis, the matrices representing the tensor and the rotation commute with each other. The two matrices have common eigenvectors. Since the eigenvectors of rotation matrix are found easily, therefore a knowledge of eigenvectors of the rotation matrix provides us with a fair amount of information about eigenvectors of the elasticity tensor. This result is first applied to a transversely isotropic tensor T of rank 2. Eigenvectors of T are found without any appeal to its components and it is also shown that due to the choice of symmetry axis as x_3 -axis, the matrix representing T is diagonal with two components equal. Then it is also applied to elasticity tensor \hat{c} possessing tetragonal symmetry to find its eigenvectors easily and also derive its classical matrix representations. The eigenvalues of \hat{c} are also found such that eigenvalues and eigenvectors are in agreement with [33] and [11] respectively. The representation of the elasticity tensor \hat{c} belonging to a particular symmetry, that is cubic, isotropic, tetragonal, hexagonal, trigonal is also derived in an elegant manner. For the cubic symmetry the representation of \hat{c} contains three parameters which, being eigenvalues of the tensor, are invariant under a coordinate transformation. Similarly for a hexagonal symmetry, it has five parameters out of which four are eigenvalues, for tetragonal symmetry, again there are seven parameters, five of them are eigenvalues and for trigonal symmetry, again there are seven parameters among which four are eigenvalues.

Chapter 4 is devoted to the identification of symmetry of an elastic materials. For the identification of plane of symmetry, Cowin and Mehrabadi [28] have proved Theorem 2.2, which is also known as Cowin-Mehrabadi Theorem. The conditions (2.52)-(2.55) of theorem 2.2 were modified by Cowin [29] and has reduced to only two conditions (2.54) and (2.55). Ting [30] has further generalized Cowin-Mehrabadi Theorem and has provided its several cases. Ahmad [31] has proved Cowin-Mehrabadi Theorem for an axis of symmetry. He has also proved Cowin-Mehrabadi Theorem in six dimensions [21]. The work done in this chapter extends the ideas of Cowin-Mehrabadi Theorem as discussed above.

In this chapter, we provide simple proofs of the necessary and sufficient conditions Cowin-Mehrabadi Theorem its special case for an axis of symmetry given in Theorem 2.2 and Theorem 2.10 respectively. This approach is generalized to a cartesian tensor of arbitrary rank and apply this treatment to find the necessary and sufficient conditions for the existence of a plane of symmetry or an axis of symmetry for a piezoelectric material. We also obtain the conditions for the identification of an *n*-fold axis of symmetry with $n \ge 3$. The necessary and sufficient conditions for the plane and axes of symmetry of elastic as well as piezoelectric tensor. These results are presented in Theorems 4.1 to Theorem 4.8. The necessary conditions for tensor of arbitrary rank is also presented at the end of the chapter.

In chapter 5, we discussed the extrema of Young's modulus for aubic and hexagonal materials. Our motivation comes from Norris [35] who has expressed the Young's modulus in term of invariant quantities, i.e. in terms of eigenvalues. On the other hand, Cazzani and Rovati [53] (also see [54], [49]) have expressed the Young's modulus in terms of the elastic compliances and the parameters which are not invariant quantities.

For extrema of Young's modulus in cubic materials, we have discussed the problem considered by Norris [35] in detail and reformulated it in six dimensions by applying the representation derived for a cubic material in chapter 3 to find an expression for $E(\mathbf{n})$. In a similar way, the expression of Young's modulus for a hexagonal material is written in terms of one variable only and hence the problem of finding extreme values is solved by a straightforward manner. The results are finally illustrated by some examples of real materials.

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