OPTIMAL ORIENTATION OF ANISOTROPIC SOLIDS

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Summary

Results are presented for finding the optimal orientation of an anisotropic elastic material. The problem is formulated as minimizing the strain energy subject to rotation of the material axes, under a state of uniform stress. It is shown that a stationary value of the strain energy requires the stress and strain tensors to have a common set of principal axes. The new derivation of this well-known coaxiality condition uses the six-dimensional expression of the rotation tensor for the elastic moduli. Using this representation it is shown that the stationary condition is a minimum or a maximum if an explicit set of conditions is satisfied. Specific results are given for materials of cubic, transversely isotropic (TI) and tetragonal symmetries. In each case the existence of a minimum or maximum depends on the sign of a single elastic constant. The stationary (minimum or maximum) value of energy can always be achieved for cubic materials. Typically, the optimal orientation of a solid with cubic material symmetry is not aligned with the symmetry directions. Expressions are given for the optimal orientation of TI and tetragonal materials, and are in agreement with results of Rovati and Taliercio obtained by a different procedure. A new concept is introduced: the strain deviation angle, which defines the degree to which a state of stress or strain is not optimal. The strain deviation angle is zero for coaxial stress and strain. An approximate formula is given for the strain deviation angle which is valid for materials that are weakly anisotropic.

1. Introduction

The strain energy of a piece of homogeneous anisotropic elastic material depends on the orientation of the material relative to the directions of principal stress, although the orientation dependence vanishes trivially for isotropic solids. This property is therefore an inherently anisotropic feature of elasticity, and it raises the question of how to find the material orientation (if any) which minimizes the strain energy for a given state of stress or strain. New results are presented in this paper on the determination of optimal orientations for both general and specific types of anisotropy.

The general problem of determining optimal orientations in anisotropic elasticity has been the subject of several studies in the last two decades, beginning with the work of Seregin and Troitskii (**1**) in the context of orthotropic solids. They determined the important *coaxiality condition*: a minimum or maximum of strain energy requires that the stress and strain share common principal axes. The coaxiality condition was subsequently and independently obtained by others: first, by Rovati and Taliercio (**2**) who considered three-dimensional elastic materials with orthotropic and cubic symmetries (although their derivation is not restricted to these symmetries but is applicable to general anisotropy), and later by Cowin (**3**). Cowin derived the coaxiality condition independent of material symmetry considerations. He showed that the commutativity of the stress and strain

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is a consequence of the stationarity condition of the strain energy with respect to rotations of the moduli. Vianello (**4**) provided a more formal derivation of coaxiality in linear elasticity. He used the tangent space of the rotation group to show that there are at least two orientations of the moduli that simultaneously make the energy stationary and stress and strain coaxial, a result later generalized to hyperelasticity (**5**) (it was subsequently shown that at least three such orientations exist for both linear elasticity (**6**) and for hyperelasticity (**7**)). There is a slight distinction between the problems considered by Cowin and by Vianello that is important to note for our purposes (**8**). Thus, Cowin (**3**) considered stress states with fixed principal directions but arbitrary amplitudes, whereas Vianello (**4**) assumed a specific state of stress. The former constraint defines a smaller set of possible elastic moduli for which coaxiality can be attained, because it requires that optimal condition be simultaneously satisfied by a family of coaxial stresses. Not surprisingly, Cowin found that only materials with orthotropic symmetry meet these conditions. In this paper the stress state is taken as given, in the same spirit as (**4**, **9**). While the emphasis here is on three-dimensional elasticity, the optimality problem has also been addressed within the context of two-dimensional elasticity (**10** to **12**). Cowin and Yang (**13**) considered a related but more general question of optimality with respect to Kelvin modes, rather than simply the freedom to orient a given material. For a more extensive review of the literature, see (**9**).

It is interesting to note that the coaxiality condition has been derived in a variety of different ways: for particular symmetries (for example, orthotropic) (**1**), using Lagrange multipliers (**3**), from general analytic considerations (**4**), and even using the six-dimensional eigenvector properties of the elasticity tensor (**14**). The derivation of the coaxiality condition presented here differs from all these previous methods. Our starting point is a representation of the rotation matrix due to Mehrabadi *et al.* (**15**). This formulation also enables derivation of conditions for minima or maxima, in a simpler and more general form than that obtained by Cowin (**3**). Section 2 begins with the problem definition and notation. The stationarity and min/max conditions are discussed in section 3. Specific conditions for particular material symmetries are derived in section 4, and we conclude in section 5 by defining the strain deviation angle, a concept which could have application in practical circumstances in anisotropic elasticity.

2. Problem definition and notation

2.1 *Optimal orientation of anisotropic solids*

Consider a fixed coordinate system $\{\mathbf{e_1},\ \mathbf{e_2},\ \mathbf{e_3}\}$ coincident with the principal axes of stress. The stress tensor is therefore $\boldsymbol{\sigma} = \sigma_{\mathrm{I}}\,\mathbf{e_1}\otimes\mathbf{e_1} + \sigma_{\mathrm{II}}\,\mathbf{e_2}\otimes\mathbf{e_2} + \sigma_{\mathrm{III}}\,\mathbf{e_3}\otimes\mathbf{e_3}$, where σ_{I}, σ_{II} and σ_{III} are the principal stresses, in no particular order. Alternative expressions for the stress include the 3×3 matrix representation,

$$\boldsymbol{\sigma} = \begin{bmatrix} \sigma_{\mathrm{I}} & 0 & 0 \\ 0 & \sigma_{\mathrm{II}} & 0 \\ 0 & 0 & \sigma_{\mathrm{III}} \end{bmatrix}, \tag{2.1}$$

and indicial† notation,

$$\sigma_{ij} = \sigma_{\mathrm{I}}\,\delta_{i1}\delta_{j1} + \sigma_{\mathrm{II}}\,\delta_{i2}\delta_{j2} + \sigma_{\mathrm{III}}\,\delta_{i3}\delta_{j3}. \tag{2.2}$$

†Lower case Latin suffices take on the values 1, 2 and 3, and the summation convention on repeated indices is assumed unless noted otherwise.

Our goal is to find the orientation or orientations which minimize the energy function for fixed stress

$$\mathcal{E} \equiv \sigma_{ij}\sigma_{kl}\, s_{ijkl}. \tag{2.3}$$

Here, s_{ijkl} are the components of the fourth-order compliance tensor relative to $\{\mathbf{e_1},\ \mathbf{e_2},\ \mathbf{e_3}\}$. Think of the material as being free to be oriented in such a way that $\mathcal{E}$ depends upon the orientation of the *material* with respect to the fixed principal axes of the stress. The material moduli for stiffness and compliance are $\mathbb{C}^{(0)}$ and $\mathbb{S}^{(0)}$ when aligned with the fixed axes. It is not necessary to specify at this stage whether or not the moduli possess any symmetry with respect to these axes. The main point is that the material is free to orient in arbitrary directions with *oriented* moduli $\mathbb{C}$ and $\mathbb{S}$ while the stress orientation remains fixed.

2.2 *Notation and tensor rotation*

Hooke's law relating stress σ_{ij} and strain ε_{ij} is

$$\sigma_{ij} = c_{ijkl}\varepsilon_{kl}, \qquad \varepsilon_{ij} = s_{ijkl}\sigma_{kl}. \tag{2.4}$$

Here c_{ijkl} denote the components of the stiffness tensor, inverse to the compliance: $c_{ijkl}s_{klpq} = I_{ijpq}$, where $I_{ijpq} = (\delta_{ip}\delta_{jq} + \delta_{iq}\delta_{jp})/2$ is the fourth-order identity tensor. The rotated elasticity components could be expressed in terms of the unrotated components $c_{ijkl}^{(0)}$ and $s_{ijkl}^{(0)}$, using Euler angles, for instance. The concise Voigt notation is used to represent the elements of the elasticity tensor in the fixed basis. Thus, the compliance is $\mathbb{S} = [S_{IJ}]$, $I, J = 1, 2, \dots, 6$, with $S_{12} = s_{1122}$, $S_{16} = s_{1112}$, $S_{44} = s_{2323}$, etc.,

$$\mathbb{S} = \begin{bmatrix} S_{11} & S_{12} & S_{13} & S_{14} & S_{15} & S_{16} \\ & S_{22} & S_{23} & S_{24} & S_{25} & S_{26} \\ & & S_{33} & S_{34} & S_{35} & S_{36} \\ & & & S_{44} & S_{45} & S_{46} \\ & \text{symmetric} & & & S_{55} & S_{56} \\ & & & & & S_{66} \end{bmatrix}. \tag{2.5}$$

An alternative representation for the elasticity tensor, closely related to (2.5), is the 6×6 matrix $\widehat{\mathbf{S}}$ with elements $[\widehat{S}_{IJ}]$ defined as

$$\widehat{\mathbf{S}} = \mathbf{T}\,\mathbb{S}\,\mathbf{T}, \quad \text{where } \mathbf{T} \equiv \begin{bmatrix} \mathbf{I} & 0 \\ 0 & \sqrt{2}\mathbf{I} \end{bmatrix}. \tag{2.6}$$

Explicitly,

$$\widehat{\mathbf{S}} \equiv \begin{bmatrix} S_{11} & S_{12} & S_{13} & \sqrt{2}S_{14} & \sqrt{2}S_{15} & \sqrt{2}S_{16} \\ S_{12} & S_{22} & S_{23} & \sqrt{2}S_{24} & \sqrt{2}S_{25} & \sqrt{2}S_{26} \\ S_{13} & S_{23} & S_{33} & \sqrt{2}S_{34} & \sqrt{2}S_{35} & \sqrt{2}S_{36} \\ \sqrt{2}S_{14} & \sqrt{2}S_{24} & \sqrt{2}S_{34} & 2S_{44} & 2S_{45} & 2S_{46} \\ \sqrt{2}S_{15} & \sqrt{2}S_{25} & \sqrt{2}S_{35} & 2S_{45} & 2S_{55} & 2S_{56} \\ \sqrt{2}S_{16} & \sqrt{2}S_{26} & \sqrt{2}S_{36} & 2S_{46} & 2S_{56} & 2S_{66} \end{bmatrix}, \tag{2.7}$$

This representation is useful in taking advantage of the fact that fourth-order elasticity tensors in three-dimensions are equivalent to a second-order symmetric tensor of six dimensions (**16**). Similar equations follow for $\mathbb{C}$ and $\widehat{\mathbf{C}} = \mathbf{T}\,\mathbb{C}\,\mathbf{T}$. Define

$$\widehat{\boldsymbol{\sigma}} \equiv (\sigma_{11},\ \sigma_{22},\ \sigma_{33},\ \sqrt{2}\sigma_{23},\ \sqrt{2}\sigma_{31},\ \sqrt{2}\sigma_{12})^T, \quad \widehat{\boldsymbol{\varepsilon}} \equiv (\varepsilon_{11},\ \varepsilon_{22},\ \varepsilon_{33},\ \sqrt{2}\varepsilon_{23},\ \sqrt{2}\varepsilon_{31},\ \sqrt{2}\varepsilon_{12})^T;$$

then the stress–strain relations (2.4) become

$$\widehat{\boldsymbol{\sigma}} = \widehat{\mathbf{C}}\widehat{\boldsymbol{\varepsilon}}, \quad \widehat{\boldsymbol{\varepsilon}} = \widehat{\mathbf{S}}\widehat{\boldsymbol{\sigma}}. \tag{2.8}$$

Note that $\widehat{\mathbf{S}}$ and $\widehat{\mathbf{C}}$ are the matrix inverse of each other; $\widehat{\mathbf{S}}\widehat{\mathbf{C}} = \widehat{\mathbf{C}}\widehat{\mathbf{S}} = \widehat{\mathbf{I}}$, where $\widehat{\mathbf{I}} = \mathrm{diag}\,(1, 1, 1, 1, 1, 1)$.

The rotation about $\mathbf{n}$, $|\mathbf{n}| = 1$ by an angle ϕ is defined as $\mathbf{Q}(\mathbf{n}, \phi) \in O(3)$, such that vectors (including the basis vectors) transform as $\mathbf{v} \to \mathbf{v}' = \mathbf{Q}\mathbf{v}$. By considering small rotations, it may be readily seen that $\mathbf{Q}(\mathbf{n}, \phi)$ can be expressed in terms of a skew symmetric tensor $\mathbf{P}$ that is linear in $\mathbf{n}$. Thus,

$$\frac{d\mathbf{Q}}{d\phi}(\mathbf{n}, \phi) = \mathbf{P}\,\mathbf{Q}(\mathbf{n}, \phi), \quad \text{where} \quad P_{ij}(\mathbf{n}) = e_{ijk}n_k, \tag{2.9}$$

and hence

$$\mathbf{Q} = e^{\phi\mathbf{P}}. \tag{2.10}$$

Note that $\mathbf{Q}$ possesses alternative well-known expressions:

$$\begin{aligned} \mathbf{Q}(\mathbf{n}, \phi) &= \mathbf{I} + \sin\phi\,\mathbf{P} + (1 - \cos\phi)\mathbf{P}^2 \\ &= \mathbf{n} \otimes \mathbf{n} + \cos\phi\,(\mathbf{I} - \mathbf{n} \otimes \mathbf{n}) + \sin\phi\,\mathbf{P}. \end{aligned} \tag{2.11}$$

In particular for our needs here, the small angle expansion is

$$\mathbf{Q}(\mathbf{n}, \phi) = \mathbf{I} + \phi\mathbf{P} + O(\phi^2)\,. \tag{2.12}$$

Under the change of basis associated with $\mathbf{Q}(\mathbf{n}, \phi)$, second-order tensors (including stress and strain) transform as $\boldsymbol{\sigma} \to \boldsymbol{\sigma}'$, where

$$\sigma'_{ij} = Q_{ir}Q_{js}\,\sigma_{rs} \Leftrightarrow \sigma'_{ij} = \mathcal{Q}_{ijrs}\,\sigma_{rs}. \tag{2.13}$$

The fourth-order 'rotation' tensor follows from (2.13) as

$$\mathcal{Q}_{ijrs} = \frac{1}{2}\left(Q_{ir}Q_{js} + Q_{is}Q_{jr}\right), \tag{2.14}$$

and (2.9) and (2.14) imply

$$\frac{d\mathcal{Q}_{ijrs}}{d\phi}(\mathbf{n}, \phi) = \mathcal{P}_{ijpq}\mathcal{Q}_{pqrs}, \quad \text{with} \quad \mathcal{Q}_{ijrs}(\mathbf{n}, 0) = I_{ijpq}, \tag{2.15}$$

where

$$\mathcal{P}_{ijpq} = \frac{1}{2}\left(\delta_{ip}P_{jq} + \delta_{iq}P_{jp} + \delta_{jp}P_{iq} + \delta_{jq}P_{ip}\right). \tag{2.16}$$

The formal solution of (2.15), with meaning that should be clear, is

$$\mathcal{Q} = e^{\phi\mathcal{P}}, \tag{2.17}$$

and the small angle approximation is

$$\mathcal{Q}_{ijpq} = I_{ijpq} + \phi\mathcal{P}_{ijpq} + O(\phi^2). \tag{2.18}$$

Mehrabadi *et al.* (**15**) derived an elegant expression for $\mathcal{Q}$ analogous to the representation for $\mathbf{Q}(\mathbf{n},\phi)$. The key is the characteristic equation of $\mathcal{P}$ ($\mathcal{P}^5 + 5\mathcal{P}^3 + 4\mathcal{P} = 0$, where $\mathcal{P}^2_{ijkl} = \mathcal{P}_{ijpq}\mathcal{P}_{pqkl}$, etc.) which permits the exponential expression (2.17) to be simplified. The result is most simply presented in terms of the 6×6 rotation matrix $\widehat{\mathbf{Q}}$ introduced by Mehrabadi *et al.* (**15**), and defined in the same manner as before. Thus, $\widehat{\mathbf{Q}} = \mathbf{T}\mathcal{Q}\mathbf{T}$ and $\widehat{\mathbf{P}} = \mathbf{T}\mathcal{P}\mathbf{T}$, where $\mathbf{T}$ is defined in (2.6) and $\mathcal{Q}$ and $\mathcal{P}$ are the 6×6 Voigt matrices. Explicitly, $\widehat{\mathbf{P}}$ is a skew symmetric six-dimensional tensor linear in $\mathbf{n}$:

$$\widehat{\mathbf{P}}(\mathbf{n}) = \begin{bmatrix} 0 & 0 & 0 & 0 & \sqrt{2}n_2 & -\sqrt{2}n_3 \\ 0 & 0 & 0 & -\sqrt{2}n_1 & 0 & \sqrt{2}n_3 \\ 0 & 0 & 0 & \sqrt{2}n_1 & -\sqrt{2}n_2 & 0 \\ 0 & \sqrt{2}n_1 & -\sqrt{2}n_1 & 0 & n_3 & -n_2 \\ -\sqrt{2}n_2 & 0 & \sqrt{2}n_2 & -n_3 & 0 & n_1 \\ \sqrt{2}n_3 & -\sqrt{2}n_3 & 0 & n_2 & -n_1 & 0 \end{bmatrix}; \tag{2.19}$$

$\widehat{\mathbf{Q}}(\mathbf{n},\phi)$ is an orthogonal second-order tensor of six dimensions, satisfying $\widehat{\mathbf{Q}}\widehat{\mathbf{Q}}^T = \widehat{\mathbf{Q}}^T\widehat{\mathbf{Q}} = \widehat{\mathbf{I}}$. Equation (2.17) becomes

$$\widehat{\mathbf{Q}}(\mathbf{n},\phi) = e^{\phi\widehat{\mathbf{P}}(\mathbf{n})}, \tag{2.20}$$

and has the explicit expansion (**15**)

$$\widehat{\mathbf{Q}}(\mathbf{n},\phi) = \widehat{\mathbf{I}} + \sin\phi\,\widehat{\mathbf{P}} + (1-\cos\phi)\,\widehat{\mathbf{P}}^2 + \frac{1}{3}\sin\phi(1-\cos\phi)\,(\widehat{\mathbf{P}}+\widehat{\mathbf{P}}^3) + \frac{1}{6}(1-\cos\phi)^2\,(\widehat{\mathbf{P}}^2+\widehat{\mathbf{P}}^4). \tag{2.21}$$

Finally, we note that fourth-order tensors $\mathbb{C}$ transform as $\widehat{\mathbf{C}} \to \widehat{\mathbf{C}}' = \widehat{\mathbf{Q}}\widehat{\mathbf{C}}\widehat{\mathbf{Q}}^T$.

2.3 *Orientation function revisited*

Denote the matrix of rotation from the fixed to the 'current' axes as $\widehat{\mathbf{Q}}$. Thus,

$$\widehat{\mathbf{C}} = \widehat{\mathbf{Q}}\widehat{\mathbf{C}}^{(0)}\widehat{\mathbf{Q}}^T, \quad \widehat{\mathbf{S}} = \widehat{\mathbf{Q}}\widehat{\mathbf{S}}^{(0)}\widehat{\mathbf{Q}}^T. \tag{2.22}$$

Hence the objective function of (2.3) for the stress-based energy minimization becomes

$$\mathcal{E} = \widehat{\boldsymbol{\sigma}}^T\,\widehat{\mathbf{S}}\,\widehat{\boldsymbol{\sigma}}\,. \tag{2.23}$$

This is the starting point in the next section to derive conditions necessary for a minimum. It is important to emphasize the initial assumption that the stress is aligned with the fixed axes, (2.1), or in terms of $\widehat{\boldsymbol{\sigma}}$,

$$\widehat{\boldsymbol{\sigma}} \equiv (\sigma_{\mathrm{I}},\ \sigma_{\mathrm{II}},\ \sigma_{\mathrm{III}},\ 0,\ 0,\ 0)^T. \tag{2.24}$$

This ensures that the energy varies as the material axes are rotated (if the stress were also rotated then the energy would be, trivially, unchanged).

3. Stationarity and min/max conditions

3.1 *Angular derivatives of the strain energy*

Consider the energy $\mathcal{E}$ of (2.23) as a function of the rotation $\widehat{\mathbf{Q}}$. A stationary value is obtained if $\mathcal{E}$ is unchanged with respect to additional small rotations of $\widehat{\mathbf{S}}$. This requires calculating the first derivative with respect to rotation angle for arbitrary rotation. The second derivative is needed to distinguish the stationary point as a minimum or maximum, or otherwise.

The strain energy obtained by arbitrary rotation of the material about the axis $\mathbf{n}$ is

$$\mathcal{E}(\mathbf{n}, \phi) = \widehat{\boldsymbol{\sigma}}^T\, \widehat{\mathbf{Q}}(\mathbf{n}, \phi)\widehat{\mathbf{S}}\widehat{\mathbf{Q}}^T(\mathbf{n}, \phi)\, \widehat{\boldsymbol{\sigma}}. \tag{3.1}$$

The first derivative can be expressed as

$$\begin{aligned}\frac{\partial}{\partial\phi}\mathcal{E}(\mathbf{n}, \phi) &= \widehat{\boldsymbol{\sigma}}^T\, \big[\widehat{\mathbf{P}}(\mathbf{n})\widehat{\mathbf{Q}}(\mathbf{n}, \phi)\widehat{\mathbf{S}}\widehat{\mathbf{Q}}^T(\mathbf{n}, \phi) + \widehat{\mathbf{Q}}(\mathbf{n}, \phi)\widehat{\mathbf{S}}^T\widehat{\mathbf{Q}}^T(\mathbf{n}, \phi)\widehat{\mathbf{P}}^T(\mathbf{n})\big]\, \widehat{\boldsymbol{\sigma}} \\ &= 2\widehat{\boldsymbol{\sigma}}^T\, \widehat{\mathbf{P}}(\mathbf{n})\widehat{\mathbf{Q}}(\mathbf{n}, \phi)\widehat{\mathbf{S}}\widehat{\mathbf{Q}}^T(\mathbf{n}, \phi)\, \widehat{\boldsymbol{\sigma}}\,. \end{aligned} \tag{3.2}$$

This follows from (2.9), (2.20) and (3.1), using the fact that $\widehat{\mathbf{P}}$ and $\widehat{\mathbf{Q}}$ commute. Similarly, the second derivative follows as

$$\frac{\partial^2}{\partial\phi^2}\mathcal{E}(\mathbf{n}, \phi) = 2\widehat{\boldsymbol{\sigma}}^T\, \big[\widehat{\mathbf{P}}^2(\mathbf{n})\widehat{\mathbf{Q}}(\mathbf{n}, \phi)\widehat{\mathbf{S}}\widehat{\mathbf{Q}}^T(\mathbf{n}, \phi) + \widehat{\mathbf{P}}(\mathbf{n})\widehat{\mathbf{Q}}(\mathbf{n}, \phi)\widehat{\mathbf{S}}\widehat{\mathbf{Q}}^T(\mathbf{n}, \phi)\widehat{\mathbf{P}}^T(\mathbf{n})\big]\, \widehat{\boldsymbol{\sigma}}\,. \tag{3.3}$$

3.2 *Condition for stationary strain energy*

Assume, with no loss in generality, that the stationary orientation is at $\phi = 0$. If $\widehat{\mathbf{S}}$ is at a stationary point, then the energy should be unchanged regardless of the axis $\mathbf{n}$, or

$$\mathcal{E} \text{ stationary} \Leftrightarrow \left.\frac{\partial}{\partial\phi}\mathcal{E}(\mathbf{n}, \phi)\right|_{\phi=0} = 0, \quad \forall\, |\mathbf{n}| = 1. \tag{3.4}$$

This becomes, using (3.2) evaluated at $\phi = 0$,

$$\left.\frac{\partial}{\partial\phi}\mathcal{E}(\mathbf{n}, \phi)\right|_{\phi=0} = 2\widehat{\boldsymbol{\sigma}}^T\, \widehat{\mathbf{P}}(\mathbf{n})\widehat{\mathbf{S}}\, \widehat{\boldsymbol{\sigma}}. \tag{3.5}$$

We now take advantage of the fact that the stress is aligned with the fixed axes. Thus, (2.19) and (2.24) give

$$\widehat{\boldsymbol{\sigma}}^T\, \widehat{\mathbf{P}}(\mathbf{n}) = (0,\ 0,\ 0,\ \sqrt{2}(\sigma_{\mathrm{III}} - \sigma_{\mathrm{II}})n_1,\ \sqrt{2}(\sigma_{\mathrm{I}} - \sigma_{\mathrm{III}})n_2,\ \sqrt{2}(\sigma_{\mathrm{II}} - \sigma_{\mathrm{I}})n_3). \tag{3.6}$$

Hence,

$$\widehat{\boldsymbol{\sigma}}^T\, \widehat{\mathbf{P}}(\mathbf{n})\widehat{\mathbf{S}}\, \widehat{\boldsymbol{\sigma}} = 2\begin{bmatrix}(\sigma_{\mathrm{III}} - \sigma_{\mathrm{II}})n_1 \\ (\sigma_{\mathrm{I}} - \sigma_{\mathrm{III}})n_2 \\ (\sigma_{\mathrm{II}} - \sigma_{\mathrm{I}})n_3\end{bmatrix}^T \begin{bmatrix} S_{14} & S_{24} & S_{34} \\ S_{15} & S_{25} & S_{35} \\ S_{16} & S_{26} & S_{36}\end{bmatrix}\begin{bmatrix}\sigma_{\mathrm{I}} \\ \sigma_{\mathrm{II}} \\ \sigma_{\mathrm{III}}\end{bmatrix}. \tag{3.7}$$

This must vanish for arbitrary direction $\mathbf{n}$, hence the energy $\mathcal{E}$ is stationary if

$$\begin{bmatrix}\sigma_{\mathrm{III}} - \sigma_{\mathrm{II}} & 0 & 0 \\ 0 & \sigma_{\mathrm{I}} - \sigma_{\mathrm{III}} & 0 \\ 0 & 0 & \sigma_{\mathrm{II}} - \sigma_{\mathrm{I}}\end{bmatrix}\begin{bmatrix} S_{14} & S_{24} & S_{34} \\ S_{15} & S_{25} & S_{35} \\ S_{16} & S_{26} & S_{36}\end{bmatrix}\begin{bmatrix}\sigma_{\mathrm{I}} \\ \sigma_{\mathrm{II}} \\ \sigma_{\mathrm{III}}\end{bmatrix} = \begin{bmatrix}0 \\ 0 \\ 0\end{bmatrix}. \tag{3.8}$$

Let us assume for simplicity that the state of stress is triaxial, so that $\sigma_{\mathrm{I}},\ \sigma_{\mathrm{II}},\ \sigma_{\mathrm{III}}$ are distinct. The left matrix in (3.8) can be removed, implying a linear condition in the stress:

$$\mathbf{E}\,\big(\sigma_{\mathrm{I}},\ \sigma_{\mathrm{II}},\ \sigma_{\mathrm{III}}\big)^T = \big(0,\ 0,\ 0\big)^T, \tag{3.9}$$

where $\mathbf{E}$ involves moduli (compliances) only

$$\mathbf{E} = \begin{bmatrix} S_{14} & S_{24} & S_{34} \\ S_{15} & S_{25} & S_{35} \\ S_{16} & S_{26} & S_{36} \end{bmatrix}. \tag{3.10}$$

Thus, the energy function $\mathcal{E}$ is stationary if $(\sigma_{\rm I},\ \sigma_{\rm II},\ \sigma_{\rm III})$ is a right null vector of the 3×3 matrix $\mathbf{E}$. Based on (2.8) and (2.1), the condition (3.9) is equivalent to the requirement that the off-diagonal elements of the strain vanish:

$$\varepsilon_{23} = \varepsilon_{31} = \varepsilon_{12} = 0 \tag{3.11}$$

or

$$\mathcal{E} \text{ stationary} \Leftrightarrow \widehat{\boldsymbol{\varepsilon}} = \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ 0 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} \varepsilon_{\rm I} \\ \varepsilon_{\rm II} \\ \varepsilon_{\rm III} \\ 0 \\ 0 \\ 0 \end{bmatrix}. \tag{3.12}$$

where $\varepsilon_{\rm I}, \varepsilon_{\rm II}, \varepsilon_{\rm III}$ are the principal strains. We have therefore derived the following simple but important general result.

RESULT 1 The energy $\mathcal{E}$ is stationary if and only if the stress and strain are coaxial.

Equation (3.11) states that the 3-vector $(\sigma_{\rm I},\ \sigma_{\rm II},\ \sigma_{\rm III})$ is a right null vector of $\mathbf{E}$. This requires as a *necessary but not sufficient condition* that

$$\det \mathbf{E} = 0. \tag{3.13}$$

Consequences of this condition were explored in detail by Rovati and Taliercio (**9**) for particular material symmetries: cubic, transversely isotropic and tetragonal. A different approach is taken in section 4 below, where the strain energy will be minimized directly.

While Result 1 is not new but has been derived by several authors (**1** to **4**, **14**, **9**), the present derivation is novel and explicit. In particular, it allows us to go further and obtain the condition necessary for a minimum or maximum. This is explored next.

3.3 *Condition for an energy minimum*

The second derivative of $\mathcal{E}$ at the stationary point follows from (3.3) evaluated at $\phi = 0$,

$$\left.\frac{\partial^2}{\partial \phi^2}\mathcal{E}(\mathbf{n},\phi)\right|_{\phi=0} = 2\widehat{\boldsymbol{\sigma}}^T \left[\widehat{\mathbf{P}}^2\widehat{\mathbf{S}} + \widehat{\mathbf{P}}\widehat{\mathbf{S}}\widehat{\mathbf{P}}^T\right]\widehat{\boldsymbol{\sigma}}. \tag{3.14}$$

Each term on the right-hand side will be examined in turn. Using (3.6), it follows that the term $\widehat{\boldsymbol{\sigma}}^T\,\widehat{\mathbf{P}}^2\widehat{\mathbf{S}}\,\widehat{\boldsymbol{\sigma}}$ is equal to

$$2\begin{bmatrix} \sigma_{\rm I} \\ \sigma_{\rm II} \\ \sigma_{\rm III} \end{bmatrix}^T \begin{bmatrix} S_{11} & S_{12} & S_{13} & S_{14} & S_{15} & S_{16} \\ S_{12} & S_{22} & S_{23} & S_{24} & S_{25} & S_{26} \\ S_{13} & S_{23} & S_{33} & S_{34} & S_{35} & S_{36} \end{bmatrix} \begin{bmatrix} (\sigma_{\rm III}-\sigma_{\rm I})n_2^2 + (\sigma_{\rm II}-\sigma_{\rm I})n_3^2 \\ (\sigma_{\rm I}-\sigma_{\rm II})n_3^2 + (\sigma_{\rm III}-\sigma_{\rm II})n_1^2 \\ (\sigma_{\rm II}-\sigma_{\rm III})n_1^2 + (\sigma_{\rm I}-\sigma_{\rm III})n_2^2 \\ (\sigma_{\rm II}+\sigma_{\rm III}-2\sigma_{\rm I})n_2n_3 \\ (\sigma_{\rm III}+\sigma_{\rm I}-2\sigma_{\rm II})n_3n_1 \\ (\sigma_{\rm I}+\sigma_{\rm II}-2\sigma_{\rm III})n_1n_2 \end{bmatrix},$$

and

$$\widehat{\boldsymbol{\sigma}}^T\, \widehat{\mathbf{P}}\widehat{\mathbf{S}}\widehat{\mathbf{P}}^T\, \widehat{\boldsymbol{\sigma}} = 4\begin{bmatrix}(\sigma_{\mathrm{III}}-\sigma_{\mathrm{II}})n_1\\(\sigma_{\mathrm{I}}-\sigma_{\mathrm{III}})n_2\\(\sigma_{\mathrm{II}}-\sigma_{\mathrm{I}})n_3\end{bmatrix}^T \begin{bmatrix}S_{44} & S_{45} & S_{46}\\ S_{45} & S_{55} & S_{56}\\ S_{46} & S_{56} & S_{66}\end{bmatrix} \begin{bmatrix}(\sigma_{\mathrm{III}}-\sigma_{\mathrm{II}})n_1\\(\sigma_{\mathrm{I}}-\sigma_{\mathrm{III}})n_2\\(\sigma_{\mathrm{II}}-\sigma_{\mathrm{I}})n_3\end{bmatrix}. \tag{3.15}$$

Thus,

$$\frac{\partial^2}{\partial\phi^2}\mathcal{E}(\mathbf{n},\phi)\bigg|_{\phi=0} = 4\,\mathbf{n}^T\mathbf{F}\mathbf{n}, \tag{3.16}$$

where the symmetric 3×3 matrix $\mathbf{F}$ has elements

$$\begin{aligned}
F_{11} &= (\sigma_{\mathrm{III}}-\sigma_{\mathrm{II}})\left[2S_{44}(\sigma_{\mathrm{III}}-\sigma_{\mathrm{II}}) + (S_{12}-S_{13})\sigma_{\mathrm{I}} + (S_{22}-S_{23})\sigma_{\mathrm{II}} + (S_{32}-S_{33})\sigma_{\mathrm{III}}\right],\\
F_{22} &= (\sigma_{\mathrm{I}}-\sigma_{\mathrm{III}})\left[2S_{55}(\sigma_{\mathrm{I}}-\sigma_{\mathrm{III}}) + (S_{13}-S_{11})\sigma_{\mathrm{I}} + (S_{23}-S_{21})\sigma_{\mathrm{II}} + (S_{33}-S_{31})\sigma_{\mathrm{III}}\right],\\
F_{33} &= (\sigma_{\mathrm{II}}-\sigma_{\mathrm{I}})\left[2S_{66}(\sigma_{\mathrm{II}}-\sigma_{\mathrm{I}}) + (S_{11}-S_{12})\sigma_{\mathrm{I}} + (S_{21}-S_{22})\sigma_{\mathrm{II}} + (S_{31}-S_{32})\sigma_{\mathrm{III}}\right],\\
F_{23} &= 2S_{56}(\sigma_{\mathrm{I}}-\sigma_{\mathrm{III}})(\sigma_{\mathrm{II}}-\sigma_{\mathrm{I}}) + \frac{1}{2}\left(\sigma_{\mathrm{II}}+\sigma_{\mathrm{III}}-2\sigma_{\mathrm{I}}\right)\left(S_{14}\sigma_{\mathrm{I}} + S_{24}\sigma_{\mathrm{II}} + S_{34}\sigma_{\mathrm{III}}\right),\\
F_{31} &= 2S_{46}(\sigma_{\mathrm{II}}-\sigma_{\mathrm{I}})(\sigma_{\mathrm{III}}-\sigma_{\mathrm{II}}) + \frac{1}{2}\left(\sigma_{\mathrm{III}}+\sigma_{\mathrm{I}}-2\sigma_{\mathrm{II}}\right)\left(S_{15}\sigma_{\mathrm{I}} + S_{25}\sigma_{\mathrm{II}} + S_{35}\sigma_{\mathrm{III}}\right),\\
F_{12} &= 2S_{45}(\sigma_{\mathrm{III}}-\sigma_{\mathrm{II}})(\sigma_{\mathrm{I}}-\sigma_{\mathrm{III}}) + \frac{1}{2}\left(\sigma_{\mathrm{I}}+\sigma_{\mathrm{II}}-2\sigma_{\mathrm{III}}\right)\left(S_{16}\sigma_{\mathrm{I}} + S_{26}\sigma_{\mathrm{II}} + S_{36}\sigma_{\mathrm{III}}\right).
\end{aligned}$$

The second derivative (3.16) must be positive for all directions $\mathbf{n}$ at an orientation where $\mathcal{E}$ is a local minimum. Noting that

$$\begin{aligned}
F_{23} &= 2S_{56}(\sigma_{\mathrm{I}}-\sigma_{\mathrm{III}})(\sigma_{\mathrm{II}}-\sigma_{\mathrm{I}}) + \frac{1}{2}\left(\sigma_{\mathrm{II}}+\sigma_{\mathrm{III}}-2\sigma_{\mathrm{I}}\right)\varepsilon_{23},\\
F_{31} &= 2S_{46}(\sigma_{\mathrm{II}}-\sigma_{\mathrm{I}})(\sigma_{\mathrm{III}}-\sigma_{\mathrm{II}}) + \frac{1}{2}\left(\sigma_{\mathrm{III}}+\sigma_{\mathrm{I}}-2\sigma_{\mathrm{II}}\right)\varepsilon_{31},\\
F_{12} &= 2S_{45}(\sigma_{\mathrm{III}}-\sigma_{\mathrm{II}})(\sigma_{\mathrm{I}}-\sigma_{\mathrm{III}}) + \frac{1}{2}\left(\sigma_{\mathrm{I}}+\sigma_{\mathrm{II}}-2\sigma_{\mathrm{III}}\right)\varepsilon_{12},
\end{aligned} \tag{3.17}$$

it follows that at a stationary point the off-diagonal elements of $\mathbf{F}$ become

$$\begin{aligned}
F_{23} &= 2S_{56}(\sigma_{\mathrm{I}}-\sigma_{\mathrm{III}})(\sigma_{\mathrm{II}}-\sigma_{\mathrm{I}}),\\
F_{31} &= 2S_{46}(\sigma_{\mathrm{II}}-\sigma_{\mathrm{I}})(\sigma_{\mathrm{III}}-\sigma_{\mathrm{II}}),\\
F_{12} &= 2S_{45}(\sigma_{\mathrm{III}}-\sigma_{\mathrm{II}})(\sigma_{\mathrm{I}}-\sigma_{\mathrm{III}}).
\end{aligned} \tag{3.18}$$

Equivalently, by pre- and post-multiplication of $\frac{1}{2}\mathbf{F}$ by the diagonal matrix diag$[(\sigma_{\mathrm{III}}-\sigma_{\mathrm{II}})^{-1}$, $(\sigma_{\mathrm{I}}-\sigma_{\mathrm{III}})^{-1}$, $(\sigma_{\mathrm{II}}-\sigma_{\mathrm{I}})^{-1}]$, it follows that $\mathbf{G}$ must be positive definite, where

$$\begin{aligned}
G_{11} &= S_{44} + \frac{1}{2}(\sigma_{\mathrm{III}}-\sigma_{\mathrm{II}})^{-1}\left[(S_{12}-S_{13})\sigma_{\mathrm{I}} + (S_{22}-S_{23})\sigma_{\mathrm{II}} + (S_{32}-S_{33})\sigma_{\mathrm{III}}\right],\\
G_{22} &= S_{55} + \frac{1}{2}(\sigma_{\mathrm{I}}-\sigma_{\mathrm{III}})^{-1}\left[(S_{13}-S_{11})\sigma_{\mathrm{I}} + (S_{23}-S_{21})\sigma_{\mathrm{II}} + (S_{33}-S_{31})\sigma_{\mathrm{III}}\right],\\
G_{33} &= S_{66} + \frac{1}{2}(\sigma_{\mathrm{II}}-\sigma_{\mathrm{I}})^{-1}\left[(S_{11}-S_{12})\sigma_{\mathrm{I}} + (S_{21}-S_{22})\sigma_{\mathrm{II}} + (S_{31}-S_{32})\sigma_{\mathrm{III}}\right],\\
G_{23} &= S_{56},\quad G_{31} = S_{46},\quad G_{12} = S_{45}.
\end{aligned} \tag{3.19}$$

Note that $G_{11} = S_{44} - \frac{1}{2}(\sigma_{\mathrm{III}} - \sigma_{\mathrm{II}})^{-1}(\varepsilon_3 - \varepsilon_2)$, etc. or, using (3.12),

$$\mathbf{G} = \begin{bmatrix} S_{44} - \dfrac{1}{2}\left(\dfrac{\varepsilon_{\mathrm{III}} - \varepsilon_{\mathrm{II}}}{\sigma_{\mathrm{III}} - \sigma_{\mathrm{II}}}\right) & S_{45} & S_{46} \\ S_{45} & S_{55} - \dfrac{1}{2}\left(\dfrac{\varepsilon_{\mathrm{I}} - \varepsilon_{\mathrm{III}}}{\sigma_{\mathrm{I}} - \sigma_{\mathrm{III}}}\right) & S_{56} \\ S_{46} & S_{56} & S_{66} - \dfrac{1}{2}\left(\dfrac{\varepsilon_{\mathrm{II}} - \varepsilon_{\mathrm{I}}}{\sigma_{\mathrm{II}} - \sigma_{\mathrm{I}}}\right) \end{bmatrix}. \tag{3.20}$$

In summary,

$$\frac{\partial^2}{\partial\phi^2}\mathcal{E}(\mathbf{n},\phi)\bigg|_{\phi=0} = 8\begin{bmatrix}(\sigma_{\mathrm{III}} - \sigma_{\mathrm{II}})n_1 \\ (\sigma_{\mathrm{I}} - \sigma_{\mathrm{III}})n_2 \\ (\sigma_{\mathrm{II}} - \sigma_{\mathrm{I}})n_3\end{bmatrix}^T \mathbf{G}\begin{bmatrix}(\sigma_{\mathrm{III}} - \sigma_{\mathrm{II}})n_1 \\ (\sigma_{\mathrm{I}} - \sigma_{\mathrm{III}})n_2 \\ (\sigma_{\mathrm{II}} - \sigma_{\mathrm{I}})n_3\end{bmatrix}. \tag{3.21}$$

This must hold for arbitrary $\mathbf{n}$, $|\mathbf{n}| = 1$, and again assuming that the principal stresses are distinct, it follows that $\mathbf{G}$ must be positive definite. Combined with Result 1 for the existence of a stationary point, this gives the next result.

RESULT 2 The energy $\mathcal{E}$ is a local minimum if the stress and strain are coaxial and the symmetric matrix $\mathbf{G}$ of (3.20) is positive definite.

This can be rewritten (with obvious notation)

$$\begin{bmatrix} S_{44} & S_{45} & S_{46} \\ S_{45} & S_{55} & S_{56} \\ S_{46} & S_{56} & S_{66}\end{bmatrix} > \begin{bmatrix} \dfrac{1}{2}\left(\dfrac{\varepsilon_{\mathrm{III}} - \varepsilon_{\mathrm{II}}}{\sigma_{\mathrm{III}} - \sigma_{\mathrm{II}}}\right) & 0 & 0 \\ 0 & \dfrac{1}{2}\left(\dfrac{\varepsilon_{\mathrm{I}} - \varepsilon_{\mathrm{III}}}{\sigma_{\mathrm{I}} - \sigma_{\mathrm{III}}}\right) & 0 \\ 0 & 0 & \dfrac{1}{2}\left(\dfrac{\varepsilon_{\mathrm{II}} - \varepsilon_{\mathrm{I}}}{\sigma_{\mathrm{II}} - \sigma_{\mathrm{I}}}\right)\end{bmatrix}. \tag{3.22}$$

The left matrix is positive definite because of the positive definite properties of the moduli. The minimum condition therefore requires that this latter matrix be greater than the right-hand diagonal matrix defined by the principal stresses and strains.‡ The requirement that the full matrix is positive definite can be relaxed if the stationarity is restricted in orientation axis $\mathbf{n}$. Thus, only the single scalar quantity $\mathbf{n}^T\mathbf{G}\mathbf{n}$ needs to be considered in the important special case of rotation about a single axis. This situation is examined in detail in the Appendix.

4. Optimal orientation of particular material symmetries

4.1 *Partition of the energy*

Before considering specific material symmetries, several general results are presented which help focus attention on the anisotropic part of the strain energy. Separate contributions to the energy function $\mathcal{E}$ of (2.3) from isotropic and anisotropic parts of the elastic moduli may be distinguished as follows:

$$\mathcal{E} = \mathcal{E}^{(\mathrm{is})} + \mathcal{E}^{(\mathrm{an})} = \sigma_{ij}\sigma_{kl}\, s_{ijkl}^{(\mathrm{is})} + \sigma_{ij}\sigma_{kl}\, s_{ijkl}^{(\mathrm{an})}. \tag{4.1}$$

‡The matrix $\mathbf{U}$ is greater than the matrix $\mathbf{V}$ if $\mathbf{r}^T\mathbf{U}\mathbf{r} > \mathbf{r}^T\mathbf{V}\mathbf{r}$ for all non-zero $\mathbf{r} \in \mathbb{R}^3$.

The moduli are partitioned into isotropic and anisotropic parts

$$s_{ijkl} = s^{(\mathrm{is})}_{ijkl} + s^{(\mathrm{an})}_{ijkl}, \quad c_{ijkl} = c^{(\mathrm{is})}_{ijkl} + c^{(\mathrm{an})}_{ijkl}, \tag{4.2}$$

with the isotropic moduli defined by

$$s^{(\mathrm{is})}_{ijkl} = \frac{1}{3\kappa_s} J_{ijkl} + \frac{1}{2\mu_s} K_{ijkl}, \quad c^{(\mathrm{is})}_{ijkl} = 3\kappa_c J_{ijkl} + 2\mu_c K_{ijkl}. \tag{4.3}$$

Here,

$$J_{ijkl} = \frac{1}{3}\delta_{ij}\delta_{kl}, \quad K_{ijkl} = I_{ijkl} - J_{ijkl}\,, \tag{4.4}$$

and I_{ijkl} are the elements of the fourth-order identity. The effective 'bulk' and 'shear' moduli $\kappa_s,\ \mu_s$ and $\kappa_c,\ \mu_c$ are obtained as

$$\frac{1}{\kappa_s} = 3s_{ijkl}J_{ijkl} = S_{11} + S_{22} + S_{33} + 2S_{12} + 2S_{13} + 2S_{23}, \tag{4.5}$$

$$\frac{15}{4\mu_s} = \frac{3}{2}s_{ijkl}K_{ijkl} = S_{11} + S_{22} + S_{33} - S_{12} - S_{23} - S_{31} + 3S_{44} + 3S_{55} + 3S_{66}, \tag{4.6}$$

$$9\kappa_c = 3c_{ijkl}J_{ijkl} = C_{11} + C_{22} + C_{33} + 2C_{12} + 2C_{13} + 2C_{23}, \tag{4.7}$$

$$15\mu_c = \frac{3}{2}c_{ijkl}K_{ijkl} = C_{11} + C_{22} + C_{33} - C_{12} - C_{23} - C_{31} + 3C_{44} + 3C_{55} + 3C_{66}. \tag{4.8}$$

Note that in general $\kappa_c \neq \kappa_s$ and $\mu_c \neq \mu_s$. The anisotropic parts of the moduli in (4.2) are defined as the remainder after subtracting the isotropic parts, $s^{(\mathrm{an})}_{ijkl} = s_{ijkl} - s^{(\mathrm{is})}_{ijkl}$, etc.

The energy associated with the isotropic part of the moduli becomes

$$\mathcal{E}^{(\mathrm{is})} = \frac{1}{\kappa_s}\overline{\sigma}^2 + \frac{1}{2\mu_s}\sigma'_{ij}\sigma'_{ij}, \tag{4.9}$$

where $\overline{\sigma}$ and $\boldsymbol{\sigma}'$ are the hydrostatic and deviatoric stress, respectively,

$$\overline{\sigma} = \frac{1}{3}\sigma_{kk}, \qquad \sigma'_{ij} = \sigma_{ij} - \overline{\sigma}\delta_{ij}. \tag{4.10}$$

These may be written explicitly in terms of the principal stresses, from (2.1), as

$$\overline{\sigma} = \frac{1}{3}\big(\sigma_{\mathrm{I}} + \sigma_{\mathrm{II}} + \sigma_{\mathrm{III}}\big),$$

$$\boldsymbol{\sigma}' = \frac{1}{3}\begin{bmatrix} 2\sigma_{\mathrm{I}} - \sigma_{\mathrm{II}} - \sigma_{\mathrm{III}} & 0 & 0 \\ 0 & 2\sigma_{\mathrm{II}} - \sigma_{\mathrm{III}} - \sigma_{\mathrm{I}} & 0 \\ 0 & 0 & 2\sigma_{\mathrm{III}} - \sigma_{\mathrm{I}} - \sigma_{\mathrm{II}} \end{bmatrix} \equiv \begin{bmatrix} \sigma'_{\mathrm{I}} & 0 & 0 \\ 0 & \sigma'_{\mathrm{II}} & 0 \\ 0 & 0 & \sigma'_{\mathrm{III}} \end{bmatrix}. \tag{4.11}$$

The energy associated with the anisotropic part of the moduli is

$$\mathcal{E}^{(\mathrm{an})} = \overline{\sigma}^2 s^{(\mathrm{an})}_{jjkk} + 2\overline{\sigma}\sigma'_{ij}\, s^{(\mathrm{an})}_{ijkk} + \sigma'_{ij}\sigma'_{kl}\, s^{(\mathrm{an})}_{ijkl}. \tag{4.12}$$

By definition, the scalar quantity $s^{(\mathrm{an})}_{jjkk}$ is zero and, accordingly, the anisotropic energy simplifies to

$$\mathcal{E}^{(\mathrm{an})} = 2\overline{\sigma}\sigma'_{ij}\, s^{(\mathrm{an})}_{ijkk} + \sigma'_{ij}\sigma'_{kl}\, s^{(\mathrm{an})}_{ijkl}. \tag{4.13}$$

It may be shown that the 3×3 matrices $\mathbf{E}$ and $\mathbf{G}$ of (3.10) and (3.20) vanish for isotropic materials. In general, they depend upon the anisotropic part of the material moduli.

4.2 *Materials with cubic symmetry*

In the fixed coordinate system of the principal stress axes, the elastic compliance for a material with cubic symmetry is

$$\mathbb{S}^{(0)} = \begin{bmatrix} S_{11}^{(0)} & S_{12}^{(0)} & S_{12}^{(0)} & 0 & 0 & 0 \\ & S_{11}^{(0)} & S_{12}^{(0)} & 0 & 0 & 0 \\ & & S_{11}^{(0)} & 0 & 0 & 0 \\ & & & S_{44}^{(0)} & 0 & 0 \\ & \text{symmetric} & & & S_{44}^{(0)} & 0 \\ & & & & & S_{44}^{(0)} \end{bmatrix}. \tag{4.14}$$

There are three independent moduli, κ, μ_1 and μ_2, where

$$\frac{1}{3\kappa} = S_{11}^{(0)} + 2S_{12}^{(0)}, \quad \frac{1}{2\mu_1} = 2S_{44}^{(0)}, \quad \frac{1}{2\mu_2} = S_{11}^{(0)} - S_{12}^{(0)}. \tag{4.15}$$

The associated fourth-order tensors can be expressed succinctly using the irreducible tensor notation of Walpole (**17**), as

$$c_{ijkl}^{(0)} = 3\kappa\, J_{ijkl} + 2\mu_1\, L_{ijkl}^{(0)} + 2\mu_2\, M_{ijkl}^{(0)}, \quad s_{ijkl}^{(0)} = \frac{1}{3\kappa}\, J_{ijkl} + \frac{1}{2\mu_1}\, L_{ijkl}^{(0)} + \frac{1}{2\mu_2}\, M_{ijkl}^{(0)}. \tag{4.16}$$

Here $L_{ijkl}^{(0)} = I_{ijkl} - D_{ijkl}^{(0)}$, $M_{ijkl}^{(0)} = D_{ijkl}^{(0)} - J_{ijkl}$, and

$$D_{ijkl}^{(0)} = \delta_{i1}\delta_{j1}\delta_{k1}\delta_{l1} + \delta_{i2}\delta_{j2}\delta_{k2}\delta_{l2} + \delta_{i3}\delta_{j3}\delta_{k3}\delta_{l3}. \tag{4.17}$$

This format makes it relatively straightforward to determine the effective isotropic moduli,

$$\kappa_c = \kappa_s = \kappa, \quad 5\mu_c = 3\mu_1 + 2\mu_2, \quad \frac{5}{\mu_s} = \frac{3}{\mu_1} + \frac{2}{\mu_2}. \tag{4.18}$$

Thus,

$$s_{ijkl}^{(\mathrm{an},0)} = \frac{1}{10}\left(\frac{1}{\mu_1} - \frac{1}{\mu_2}\right)(5J_{ijkl} + 2K_{ijkl} - 5D_{ijkl}^{(0)}). \tag{4.19}$$

The anisotropic part of the energy, (4.13), depends only upon the deviatoric part of the stress,

$$\mathcal{E}^{(\mathrm{an})} = \sigma'_{ij}\sigma'_{kl}\, s_{ijkl}^{(\mathrm{an})}. \tag{4.20}$$

The reason is that the second-order tensor $s_{ijkk}^{(\mathrm{an},0)}$ is identically zero for cubic symmetry, and hence remains zero in the rotated material axes: $s_{ijkk}^{(\mathrm{an})} = 0$. The first term in (4.13) therefore vanishes, leaving the simpler expression (4.20). The isotropic tensors J_{ijkl} and K_{ijkl} are unchanged under rotation and, consequently, from (4.9), (4.19) and (4.20),

$$\mathcal{E} = \frac{1}{\kappa}\bar{\sigma}^2 + \frac{1}{2\mu_1}\sigma'_{ij}\sigma'_{ij} + \mathcal{E}^{(\mathrm{ex})}, \qquad \mathcal{E}^{(\mathrm{ex})} = \frac{1}{2}\left(\frac{1}{\mu_2} - \frac{1}{\mu_1}\right)\sigma'_{ij}\sigma'_{kl}\, D_{ijkl}, \tag{4.21}$$

where D_{ijkl} is the rotated version of $D^{(0)}_{ijkl}$. In order to avoid ambiguity, let $\sigma_{(\mathrm{rot})kl}$ denote the stress in the *rotated* coordinate system, then it follows that

$$\sigma'_{ij}\sigma'_{kl}\,D_{ijkl} = \sigma'^{2}_{(\mathrm{rot})11} + \sigma'^{2}_{(\mathrm{rot})22} + \sigma'^{2}_{(\mathrm{rot})33}. \tag{4.22}$$

The scalar second invariant of the deviatoric stress is

$$\begin{aligned}\sigma'_{ij}\sigma'_{ij} &= \sigma'^{2}_{\mathrm{I}} + \sigma'^{2}_{\mathrm{II}} + \sigma'^{2}_{\mathrm{III}}\\ &= \sigma'^{2}_{(\mathrm{rot})11} + \sigma'^{2}_{(\mathrm{rot})22} + \sigma'^{2}_{(\mathrm{rot})33} + 2\sigma'^{2}_{(\mathrm{rot})23} + 2\sigma'^{2}_{(\mathrm{rot})31} + 2\sigma'^{2}_{(\mathrm{rot})12}.\end{aligned} \tag{4.23}$$

Therefore, the function $\mathcal{E}^{(\mathrm{ex})}$ of (4.21) is stationary when either the right member of (4.22) or

$$\Gamma = \sigma'^{2}_{(\mathrm{rot})23} + \sigma'^{2}_{(\mathrm{rot})31} + \sigma'^{2}_{(\mathrm{rot})12} \tag{4.24}$$

is stationary. Furthermore,

$$\mathcal{E}^{(\mathrm{ex})} = \mathcal{E}^{(\mathrm{ex},0)} + \left(\frac{1}{\mu_1} - \frac{1}{\mu_2}\right)\left[\sigma'^{2}_{(\mathrm{rot})23} + \sigma'^{2}_{(\mathrm{rot})31} + \sigma'^{2}_{(\mathrm{rot})12}\right], \tag{4.25}$$

where $\mathcal{E}^{(\mathrm{ex},0)}$ is the unrotated or fixed value, which follows from (4.11) as

$$\mathcal{E}^{(\mathrm{ex},0)} = \frac{1}{2}\left(\frac{1}{\mu_2} - \frac{1}{\mu_1}\right)\left(\sigma'^{2}_{\mathrm{I}} + \sigma'^{2}_{\mathrm{II}} + \sigma'^{2}_{\mathrm{III}}\right). \tag{4.26}$$

Hence,

$$\mu_1 > \mu_2 \quad \Rightarrow \quad \mathcal{E}^{(\mathrm{ex})} \leqslant \mathcal{E}^{(\mathrm{ex},0)}, \tag{4.27}$$

with equality when the material and stress axes are aligned. Thus, a local minimum that is not aligned with the stress axes occurs if and only if $\mu_1 > \mu_2$ and occurs when Γ of (4.24) achieves a local maximum. It will be shown below that the maximum value is $\frac{1}{2}\sigma'_{ij}\sigma'_{ij}$ or, equivalently, that $\mathcal{E}^{(\mathrm{ex})}$ is zero at the stationary point.

As the material axes are rotated to transform $s^{(\mathrm{an},0)}_{ijkl} \to s^{(\mathrm{an})}_{ijkl}$, the only part that contributes to the anisotropic strain energy is $D^{(0)}_{ijkl} \to D_{ijkl}$. Conditions for obtaining the stationary value of strain energy are next derived by focusing on the dependence upon D_{ijkl}. The 6×6 matrix associated with the unrotated tensor $D^{(0)}_{ijkl}$ is

$$\widehat{\mathbf{D}}^{(0)} = \begin{bmatrix} I_{3\times3} & 0_{3\times3} \\ 0_{3\times3} & 0_{3\times3}\end{bmatrix}. \tag{4.28}$$

It is convenient to split $\widehat{\mathbf{Q}}$ as follows into 3×3 matrices:

$$\widehat{\mathbf{Q}} = \begin{bmatrix} \widehat{\mathbf{Q}}_1 & \widehat{\mathbf{Q}}_2 \\ \widehat{\mathbf{Q}}_3 & \widehat{\mathbf{Q}}_4\end{bmatrix}, \tag{4.29}$$

so that the rotated tensor $\widehat{\mathbf{D}} = \widehat{\mathbf{Q}}\widehat{\mathbf{D}}^{(0)}\widehat{\mathbf{Q}}^T$ follows from (4.28) and (4.29) as

$$\widehat{\mathbf{D}} = \begin{bmatrix} \widehat{\mathbf{Q}}_1\widehat{\mathbf{Q}}_1^T & \widehat{\mathbf{Q}}_1\widehat{\mathbf{Q}}_3^T \\ \widehat{\mathbf{Q}}_3\widehat{\mathbf{Q}}_1^T & \widehat{\mathbf{Q}}_3\widehat{\mathbf{Q}}_3^T\end{bmatrix}. \tag{4.30}$$

The term associated with the rotated energy follows from (2.24) and (4.30) as

$$\sigma'_{ij}\sigma'_{kl}\, D_{ijkl} = (\sigma'_{\mathrm{I}},\ \sigma'_{\mathrm{II}},\ \sigma'_{\mathrm{III}})\, \widehat{\mathbf{Q}}_1 \widehat{\mathbf{Q}}_1^T\, (\sigma'_{\mathrm{I}},\ \sigma'_{\mathrm{II}},\ \sigma'_{\mathrm{III}})^T. \tag{4.31}$$

Thus, any stress that is a null vector of $\widehat{\mathbf{Q}}_1^T$ also yields the minimum or maximum value for $\mathcal{E}^{(\mathrm{ex})}$ of (4.21), that is, zero. This suggests $\widehat{\mathbf{Q}}_1$ as the focus of attention, and implies the following important result. Every stress state which is a null vector of $\widehat{\mathbf{Q}}_1^T$ corresponds to a global minimum (maximum) of $\mathcal{E}$ if $\mu_1 > \mu_2$ ($\mu_2 > \mu_1$). We therefore search for null vectors of $\widehat{\mathbf{Q}}_1^T$.

Before deriving two alternative methods to find null vectors of $\widehat{\mathbf{Q}}_1^T$ in the next two subsections, note that the quantity (4.22) vanishes at a stationary orientation, and hence $\sigma_{(\mathrm{rot})11} = \sigma_{(\mathrm{rot})22} = \sigma_{(\mathrm{rot})22}$. Thus, the stresses in each of the three rotated axial directions are equal, a result previously obtained by Rovati and Taliercio (**2**, **9**). Furthermore, at the stationary point it may be easily shown that the following identities hold:

$$\mathcal{D}\boldsymbol{\sigma} = \overline{\sigma}\,\mathbf{I}, \quad \mathcal{L}\boldsymbol{\sigma} = \boldsymbol{\sigma}', \quad \mathcal{M}\boldsymbol{\sigma} = 0, \tag{4.32}$$

where $\mathcal{D}$, $\mathcal{L}$, $\mathcal{M}$ are the (rotated) tensors with components D_{ijkl}, L_{ijkl}, M_{ijkl}, respectively. Hence, the strain at optimal orientation is simply

$$\boldsymbol{\varepsilon} = \frac{1}{3\kappa}\,\overline{\sigma}\,\mathbf{I} + \frac{1}{2\mu_1}\,\boldsymbol{\sigma}' \quad \text{(optimal orientation only)}. \tag{4.33}$$

This is clearly coaxial with the stress, which follows from the commutation property of coaxial second-order tensors ($\boldsymbol{\sigma\varepsilon} - \boldsymbol{\varepsilon\sigma} = 0$ in this case).

It is also worth remarking that we do not seek null vectors of the matrix $\mathbf{E}$, although this approach is feasible and has been used to advantage by Rovati and Taliercio (**9**). Some comments on $\mathbf{E}$ are in order though. The 3×3 matrix follows from (4.28) to (4.30) as

$$\mathbf{E} = \widehat{\mathbf{Q}}_3 \widehat{\mathbf{Q}}_1^T, \tag{4.34}$$

and the condition (3.13) is satisfied if either $\det \widehat{\mathbf{Q}}_1$ or $\det \widehat{\mathbf{Q}}_3$ vanishes. These can be made more explicit in terms of the elements of the rotation matrix. Let

$$\mathbf{Q} = \begin{bmatrix} q_{11} & q_{12} & q_{13} \\ q_{21} & q_{22} & q_{23} \\ q_{31} & q_{32} & q_{33} \end{bmatrix}, \tag{4.35}$$

then using the the explicit representation of the 6×6 rotation matrix from Auld (**18**) or otherwise, the condition (3.13) implies

$$\det \widehat{\mathbf{Q}}_1 = \begin{vmatrix} q_{11}^2 & q_{12}^2 & q_{13}^2 \\ q_{21}^2 & q_{22}^2 & q_{23}^2 \\ q_{31}^2 & q_{32}^2 & q_{33}^2 \end{vmatrix} = 0 \quad \text{or} \quad \det \widehat{\mathbf{Q}}_3 = 2^{\frac{3}{2}} \begin{vmatrix} q_{21}q_{31} & q_{22}q_{32} & q_{23}q_{33} \\ q_{31}q_{11} & q_{32}q_{12} & q_{33}q_{13} \\ q_{11}q_{21} & q_{12}q_{22} & q_{13}q_{23} \end{vmatrix} = 0. \tag{4.36}$$

Using the fact that the column vectors of a transformation matrix form an orthonormal triad, it follows that

$$\widehat{\mathbf{Q}}_1^T\,(1,\ 1,\ 1)^T = (1,\ 1,\ 1)^T, \quad \widehat{\mathbf{Q}}_3\,(1,\ 1,\ 1)^T = (0,\ 0,\ 0)^T. \tag{4.37}$$

That is, $(\sigma_{\mathrm{I}},\ \sigma_{\mathrm{II}},\ \sigma_{\mathrm{III}}) = \lambda\,(1,\ 1,\ 1)$ is a null vector of $\mathbf{E}$ for any λ. Hence, $\mathbf{E}$ is not of full rank, implying that $\det \mathbf{E}$ is always zero. However, this is not of interest as the null space corresponds to hydrostatic stress, for which the energy function is independent of material orientation. The implications of (4.36) are not considered further, and we return to the simpler task of finding null vectors of $\widehat{\mathbf{Q}}_1^T$ alone.

Two methods for achieving the minimum energy $\mathcal{E}^{(\mathrm{ex})} = 0$ are described, both using explicit forms of the rotation. The first involves a single rotation about an arbitrary axis, and the second is in terms of standard Euler angles.

4.2.1 *Minimum energy state with a single rotation.* The range of transformations which correspond to energy minima can be obtained using Euler's theorem (**20**) which states that any transformation matrix $\mathbf{Q}$ can be represented in the form (2.10) for some axis $\mathbf{n}$, $|\mathbf{n}| = 1$, and angle ϕ. Thus

$$\mathbf{Q}(\mathbf{n}, \phi) = \begin{bmatrix} 1 - 2s^2(n_2^2 + n_3^2) & 2s(sn_1n_2 - cn_3) & 2s(sn_1n_3 + cn_2) \\ 2s(sn_1n_2 + cn_3) & 1 - 2s^2(n_3^2 + n_1^2) & 2s(sn_2n_3 - cn_1) \\ 2s(sn_1n_3 - cn_2) & 2s(sn_2n_3 + cn_1) & 1 - 2s^2(n_1^2 + n_2^2) \end{bmatrix}, \tag{4.38}$$

where $c = \cos(\phi/2)$, $s = \sin(\phi/2)$ and the elements of the associated $\widehat{\mathbf{Q}}_1$ are determined by squaring each element in (4.38). It may be shown that

$$\det \widehat{\mathbf{Q}}_1(\mathbf{n}, \phi) = \cos 2\phi + 2(2 + 3\cos\phi)(1 - \cos\phi)^2(n_1^2n_2^2 + n_2^2n_3^2 + n_3^2n_1^2) + 6(1 - \cos\phi)^3 n_1^2n_2^2n_3^2.$$

Note that $n_1^2n_2^2 + n_2^2n_3^2 + n_3^2n_1^2 \leqslant 1/3$ and $n_1^2n_2^2n_3^2 \leqslant 1/27$ with equality when $n_1^2 = n_2^2 = n_3^2 = 1/3$.

For a given n_3^2 and angle ϕ,

$$n_1^2, n_2^2 = \tfrac{1}{2}(1 - n_3^2) \pm \left[\tfrac{1}{4}(1 - n_3^2)^2 - g\right]^{1/2}, \tag{4.39}$$

where

$$g(n_3^2, \phi) = \frac{-\cos 2\phi - 2(2 + 3\cos\phi)(1 - \cos\phi)^2\, n_3^2(1 - n_3^2)}{2(1 - \cos\phi)^2[(2 + 3n_3^2 + 3\cos\phi(1 - n_3^2)]}. \tag{4.40}$$

The null vector of $\widehat{\mathbf{Q}}_1$ is such that

$$\begin{aligned} \sigma_{\mathrm{I}}' Q_{11}^2 + \sigma_{\mathrm{II}}' Q_{12}^2 + \sigma_{\mathrm{III}}' Q_{13}^2 &= 0, \\ \sigma_{\mathrm{I}}' Q_{21}^2 + \sigma_{\mathrm{II}}' Q_{22}^2 + \sigma_{\mathrm{III}}' Q_{23}^2 &= 0, \\ \sigma_{\mathrm{I}}' Q_{31}^2 + \sigma_{\mathrm{II}}' Q_{32}^2 + \sigma_{\mathrm{III}}' Q_{33}^2 &= 0. \end{aligned} \tag{4.41}$$

Using the fact that this is a deviatoric stress, we replace $\sigma_{\mathrm{III}}' = -\sigma_{\mathrm{I}}' - \sigma_{\mathrm{II}}'$ in the final equation of (4.41), to get

$$\sigma_{\mathrm{I}}' \left(Q_{31}^2 - Q_{33}^2\right) + \sigma_{\mathrm{II}}' \left(Q_{32}^2 - Q_{33}^2\right) = 0. \tag{4.42}$$

Hence,

$$\sigma_{\mathrm{I}}' = a_0 \left(Q_{32}^2 - Q_{33}^2\right), \quad \sigma_{\mathrm{II}}' = a_0 \left(Q_{33}^2 - Q_{31}^2\right) \tag{4.43}$$

for arbitrary $a_0 \neq 0$. Once again using the fact that $\sigma_{\mathrm{III}}' = -\sigma_{\mathrm{I}}' - \sigma_{\mathrm{II}}'$ gives

$$\sigma_{\mathrm{III}}' = a_0 \left(Q_{31}^2 - Q_{32}^2\right). \tag{4.44}$$

In the same way, using the other equations in (4.41), three alternative expressions for the null vector are found:

$$\begin{aligned}\left(\sigma'_{\mathrm{I}},\ \sigma'_{\mathrm{II}},\ \sigma'_{\mathrm{III}}\right) &= a_1\left(Q_{32}^2 - Q_{32}^2,\ Q_{33}^2 - Q_{31}^2,\ Q_{31}^2 - Q_{32}^2\right)\\ &= a_2\left(Q_{12}^2 - Q_{12}^2,\ Q_{13}^2 - Q_{11}^2,\ Q_{11}^2 - Q_{12}^2\right)\\ &= a_3\left(Q_{22}^2 - Q_{22}^2,\ Q_{23}^2 - Q_{21}^2,\ Q_{21}^2 - Q_{22}^2\right)\end{aligned}$$

for some constants a_1, a_2, a_3. Thus, from the first expression, with $a_1 = 1$,

$$\sigma'_{\mathrm{I}} = \left[(1+n_1^2)(n_2^2 - n_3^2)(1-\cos\phi) + n_3^2 - n_2^2 - 4n_1n_2n_3\sin\phi\right](1-\cos\phi), \tag{4.45}$$

$$\begin{aligned}\sigma'_{\mathrm{II}} = \big\{&[(1-n_1^2)(n_1^2-n_3^2) - 2n_2^2](1-\cos\phi) + n_2^2 - n_1^2 + 1\\ &+ 2n_1n_2n_3\sin\phi\big\}(1-\cos\phi) - 1,\end{aligned} \tag{4.46}$$

$$\begin{aligned}\sigma'_{\mathrm{III}} = \big\{&[(1-n_1^2)(n_2^2-n_1^2) + 2n_3^2](1-\cos\phi) + n_1^2 - n_3^2 - 1\\ &+ 2n_1n_2n_3\sin\phi\big\}(1-\cos\phi) + 1.\end{aligned} \tag{4.47}$$

These equations provide a two-parameter set of stress states, described by $0 < n_3^2 < 1$ and ϕ. The two are independent insofar as n_1^2 and n_2^2 of (4.39) lie in (0, 1). This in turn requires that g of (4.40) satisfies

$$0 \leqslant g(n_3^2, \phi) \leqslant \frac{1}{4}(1-n_3^2)^2, \tag{4.48}$$

which defines the range of $0 < n_3^2 < 1$ and ϕ.

4.2.2 *Minimum energy using Euler angles.* The standard three Euler angles $(\theta_1,\ \theta_2,\ \theta_3)$ are used to transform from $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\} \to \{\mathbf{e}'_1, \mathbf{e}'_2, \mathbf{e}'_3 = \mathbf{e}_3\} \to \{\mathbf{e}''_1 = \mathbf{e}'_1, \mathbf{e}''_2, \mathbf{e}''_3\} \to \{\mathbf{e}'''_1, \mathbf{e}'''_2, \mathbf{e}'''_3 = \mathbf{e}''_3\}$. That is, first rotate about the $\mathbf{e}_3$ axis by θ_1, then about the $\mathbf{e}'_1$ axis by θ_2, and finally about the $\mathbf{e}''_3$ axis by θ_3. The transformation matrix, $\mathbf{Q}(\theta_1, \theta_2, \theta_3)$, is equal to

$$\begin{bmatrix}\cos\theta_1\cos\theta_3 - \sin\theta_1\cos\theta_2\sin\theta_3 & \sin\theta_1\cos\theta_3 + \cos\theta_1\cos\theta_2\sin\theta_3 & \sin\theta_2\sin\theta_3\\ -\cos\theta_1\sin\theta_3 - \sin\theta_1\cos\theta_2\cos\theta_3 & -\sin\theta_1\sin\theta_3 + \cos\theta_1\cos\theta_2\cos\theta_3 & \sin\theta_2\cos\theta_3\\ \sin\theta_1\sin\theta_2 & -\cos\theta_1\sin\theta_2 & \cos\theta_2\end{bmatrix},$$

and it follows from this and $(4.36)_1$ that

$$\det\widehat{\mathbf{Q}}_1(\theta_1, \theta_2, \theta_3) = \cos 2\theta_1\ \cos 2\theta_2\ \cos 2\theta_3 - \frac{1}{4}\ \sin 2\theta_1\ \sin 2\theta_3\ \cos\theta_2\,(3\cos 2\theta_2 + 1). \tag{4.49}$$

The condition that this vanish is equivalent to Rovati and Taliercio (**9**, equation (90)), although their result is obtained in a different manner.

Consider, for instance, $\theta_3 = 0$, for which

$$\det\widehat{\mathbf{Q}}_1(\theta_1, \theta_2, 0) = \cos 2\theta_1\ \cos 2\theta_2, \tag{4.50}$$

and hence there are null spaces associated with $\widehat{\mathbf{Q}}_1(\theta_1, \pi/4, 0)$ and $\widehat{\mathbf{Q}}_1(\pi/4, \theta_2, 0)$. The null spaces are lines in the stress space, which follow from the simplified form of $\widehat{\mathbf{Q}}_1^T$,

$$\widehat{\mathbf{Q}}_1^T(\theta_1, \theta_2, 0) = \begin{bmatrix}\cos^2\theta_1 & \sin^2\theta_1\cos^2\theta_2 & \sin^2\theta_1\sin^2\theta_2\\ \sin^2\theta_1 & \cos^2\theta_1\cos^2\theta_2 & \cos^2\theta_1\sin^2\theta_2\\ 0 & \sin^2\theta_2 & \cos^2\theta_2\end{bmatrix}. \tag{4.51}$$

The possible states of deviatoric stress are: $(\sigma_{\mathrm{I}}', \sigma_{\mathrm{II}}', \sigma_{\mathrm{III}}') = \lambda\,(0, -1, 1)$ if $\theta_2 = \pi/4$, $\theta_3 = 0$, and $(\sigma_{\mathrm{I}}', \sigma_{\mathrm{II}}', \sigma_{\mathrm{III}}') = \lambda\,(\cos 2\theta_2, -\cos^2\theta_2, \sin^2\theta_2)$ if $\theta_1 = \pi/4$, $\theta_3 = 0$. The first family of stresses correspond to a two-dimensional elasticity problem (see the Appendix): $\sigma_{\mathrm{I}}' = 0$, $\sigma_{\mathrm{II}}' + \sigma_{\mathrm{III}}' = 0$, and it is also a null vector of $\widehat{\mathbf{Q}}_1(0, \pi/4, \theta_3)$. The second is also a null vector of $\widehat{\mathbf{Q}}_1(0, \theta_2, \pi/4)$. Similarly, $\lambda\,(1, -1, 0)$ is a null vector of $\widehat{\mathbf{Q}}_1(\pi/4, \pi/2, \theta_3)$ and $\lambda\,(-\cos^2\theta_1, \sin^2\theta_1, \cos 2\theta_1)$ is a null vector of $\widehat{\mathbf{Q}}_1(\theta_1, \pi/2, \pi/4)$.

Conversely, an orientation which provides a minimum in energy can be found for a given state of stress. Assume with no loss in generality that $\sigma_{\mathrm{II}}' < 0 < \sigma_{\mathrm{III}}'$. Define the angle θ_2 by

$$\tan^2\theta_2 = -\sigma_{\mathrm{III}}'/\sigma_{\mathrm{II}}', \tag{4.52}$$

then the deviatoric stress may be expressed as

$$(\sigma_{\mathrm{I}}', \sigma_{\mathrm{II}}', \sigma_{\mathrm{III}}') = \left(\sigma_{\mathrm{III}}' - \sigma_{\mathrm{II}}'\right)(\cos 2\theta_2, -\cos^2\theta_2, \sin^2\theta_2). \tag{4.53}$$

It follows from the above example that this deviatoric stress is a null vector of $\widehat{\mathbf{Q}}_1(\pi/4, \theta_2, 0)$.

It is instructive to examine further the example (4.53). The rotated material axes, denoted by $\{\mathbf{e}_1', \mathbf{e}_2', \mathbf{e}_3'\}$, are given by the columns of $\mathbf{Q}(\pi/4, \theta_2, 0)$:

$$\mathbf{e}_1' = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ -c \\ s \end{bmatrix}, \quad \mathbf{e}_2' = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ c \\ -s \end{bmatrix}, \quad \mathbf{e}_3' = \begin{bmatrix} 0 \\ s \\ c \end{bmatrix}, \tag{4.54}$$

where $s = \sin\theta_2$, $c = \cos\theta_2$, or from (4.52),

$$s = \sqrt{\frac{\sigma_{\mathrm{III}}'}{\sigma_{\mathrm{III}}' - \sigma_{\mathrm{II}}'}}, \quad c = \sqrt{\frac{-\sigma_{\mathrm{II}}'}{\sigma_{\mathrm{III}}' - \sigma_{\mathrm{II}}'}}. \tag{4.55}$$

The rotated tensor D_{ijkl} is

$$\mathcal{D} = \mathbf{e}_1' \otimes \mathbf{e}_1' \otimes \mathbf{e}_1' \otimes \mathbf{e}_1' + \mathbf{e}_2' \otimes \mathbf{e}_2' \otimes \mathbf{e}_2' \otimes \mathbf{e}_2' + \mathbf{e}_3' \otimes \mathbf{e}_3' \otimes \mathbf{e}_3' \otimes \mathbf{e}_3', \tag{4.56}$$

and hence

$$\mathcal{D}\boldsymbol{\sigma}' = \sum_{k=1}^{3} \mathbf{e}_k' \otimes \mathbf{e}_k'\,(\mathbf{e}_k' \cdot \boldsymbol{\sigma}'\mathbf{e}_k'). \tag{4.57}$$

It may be seen by direct calculation that the three scalars $\mathbf{e}_k' \cdot \boldsymbol{\sigma}'\mathbf{e}_k'$ (no sum) are identically zero by virtue of (4.54) and (4.55). This demonstrates explicitly that

$$\mathcal{D}\boldsymbol{\sigma}' = 0 \tag{4.58}$$

at the optimal orientation. The identities (4.32) follow accordingly.

4.2.3 *Summary for cubic symmetry.* The extreme values of the energy for cubic materials are $\mathcal{E}_1$ and $\mathcal{E}_2$, where

$$\mathcal{E}_j = \frac{1}{\kappa}\bar{\sigma}^2 + \frac{1}{2\mu_j}(\sigma_{\mathrm{I}}'^2 + \sigma_{\mathrm{II}}'^2 + \sigma_{\mathrm{III}}'^2), \quad j = 1, 2. \tag{4.59}$$

The fixed axes are always one of the stationary orientations, since $\mathbf{E}$ of (3.10) vanishes. The stationary value for the unrotated axes is $\mathcal{E}_2$, which is the global minimum (maximum) if $\mu_2 > \mu_1$

($\mu_2 < \mu_1$). The stationary value $\mathcal{E}_1$ occurs at some rotated axes, the existence of which is not in doubt for a material of cubic symmetry (or any material symmetry for that matter). The important point to note is that it is possible to explicitly determine such orientations. Thus, we have shown by direct construction the material orientation that achieves the stationary energy value $\mathcal{E}_1$ for any state of stress. This is a global minimum (maximum) if $\mu_2 < \mu_1$ ($\mu_2 > \mu_1$).

It is interesting that the expressions for the extreme values in (4.59) have the form of the energy for an isotropic solid, but with different shear moduli. This is evident by writing $\mathcal{E}_1$ and $\mathcal{E}_2$ in terms of the invariants of the stress tensor:

$$\mathcal{E}_j = \frac{1}{9\kappa}(\mathrm{tr}\,\boldsymbol{\sigma})^2 + \frac{1}{2\mu_j}\left[\mathrm{tr}\,\boldsymbol{\sigma}^2 - \frac{1}{3}(\mathrm{tr}\,\boldsymbol{\sigma})^2\right], \quad j = 1,\ 2. \tag{4.60}$$

4.2.4 *Example materials.* Noting that $\mu_1 = c_{44}$ and $\mu_2 = (c_{11} - c_{12})/2$ allows us to determine the sign of $(\mu_2 - \mu_1)$. Musgrave's (**19**, Table A.1) provides data for $c^* = 2(\mu_2 - \mu_1)$ for a multitude of materials. These show c^* to be negative for most elemental and engineering materials with cubic symmetry and different lattice structures: aluminum, nickel, copper, silver, gold (all f.c.c. structure), iron (b.c.c.), brass (f.c.c. and b.c.c.), diamond, silicon, germanium (all diamond structure), and GaSb, InSb (both zinc-blende). Hence, for all of these cubic materials there exist optimal orientations of the axes that achieve the lowest energy state possible. Materials with positive c^* include crystalline compounds of potassium, sodium and silver with rock-salt structure: KF, KCL, KBr, KI, NaF, NaCl, NaBr, NaI, AgCl, AgBr; plus caesium compounds with structure related to b.c.c. For these, the orientation associated with (4.53), for instance, gives maximum strain energy. The minimum energy is achieved by no rotation.

4.3 *Transverse isotropy*

Materials with hexagonal symmetry, or equivalently, transverse isotropy (TI), are characterized by five moduli. In the coordinate system of the principal axes, the elements of the compliance are

$$\mathbb{S}^{(0)} = \begin{bmatrix} S_{11}^{(0)} & S_{12}^{(0)} & S_{13}^{(0)} & 0 & 0 & 0 \\ & S_{11}^{(0)} & S_{13}^{(0)} & 0 & 0 & 0 \\ & & S_{33}^{(0)} & 0 & 0 & 0 \\ & & & S_{44}^{(0)} & 0 & 0 \\ & \text{symmetric} & & & S_{44}^{(0)} & 0 \\ & & & & & S_{66}^{(0)} \end{bmatrix}, \tag{4.61}$$

with $S_{66}^{(0)} = \frac{1}{2}(S_{11}^{(0)} - S_{12}^{(0)})$. The TI material is characterized by an axis of symmetry, defined by the unit vector $\mathbf{n}$, which is here chosen as the $\mathbf{e}_3$ axis. In general, the strain energy depends only upon the orientation of $\mathbf{n}$ with respect to the stress axes, and the problem is formulated as one of selecting $\mathbf{n}$ to minimize $\mathcal{E}$.

First note that two of the five moduli can be ascribed to the isotropic part of the elasticity; or conversely, an isotropic part may be subtracted from the compliance tensor s_{ijkl} according to (4.2), (4.3) and (4.5), where

$$\frac{1}{\kappa_s} = 2S_{11}^{(0)} + S_{33}^{(0)} + 2S_{12}^{(0)} + 4S_{13}^{(0)}, \quad \frac{15}{4\mu_s} = 2S_{11}^{(0)} + S_{33}^{(0)} - S_{12}^{(0)} - 2S_{13}^{(0)} + 6S_{44}^{(0)} + 3S_{66}^{(0)}, \tag{4.62}$$

leaving a tensor $s^{(\mathrm{an})}_{ijkl}$ with three constants. The anisotropic compliance depends upon the orientation of the axis of symmetry as follows:

$$s^{(\mathrm{an})}_{ijkl} = a\, n_i n_j n_k n_l + b\,(\delta_{ij} n_k n_l + \delta_{kl} n_i n_j) + \frac{c}{2}\,(\delta_{ik} n_j n_l + \delta_{il} n_j n_k + \delta_{jk} n_i n_l + \delta_{jl} n_i n_k)$$
$$- \frac{1}{3}(a + 6b + 2c) J_{ijkl} - \frac{2}{15}(a + 5c) K_{ijkl}. \tag{4.63}$$

The tensors J_{ijkl} and K_{ijkl} are defined in (4.4), and the elastic constants a, b and c follow from (4.61) to (4.63) as

$$a = S^{(0)}_{11} + S^{(0)}_{33} - 2S^{(0)}_{13} - 4S^{(0)}_{44}, \quad b = S^{(0)}_{13} - S^{(0)}_{12}, \quad c = 2S^{(0)}_{44} - 2S^{(0)}_{66}. \tag{4.64}$$

The stress is, as usual, aligned with the fixed axes, so that the total strain energy follows from (4.1), (4.63) and (2.2), as

$$\mathcal{E} = \left[\frac{1}{\kappa_s} - \frac{1}{3}(a + 4b + 2c)\right] \overline{\sigma}^{\,2} + \left[\frac{1}{2\mu_s} - \frac{2}{15}(a + b + 5c)\right] \sigma'_{ij}\sigma'_{ij} + \mathcal{E}^{(\mathrm{ex})}, \tag{4.65}$$

where $\overline{\sigma}$ is defined in (4.10) and the extra energy term is

$$\mathcal{E}^{(\mathrm{ex})} = a\left(\sigma_{\mathrm{I}} n_1^2 + \sigma_{\mathrm{II}} n_2^2 + \sigma_{\mathrm{III}} n_3^2\right)^2 + (3b\overline{\sigma} + c\sigma_{\mathrm{I}})2\sigma_{\mathrm{I}} n_1^2 + (3b\overline{\sigma} + c\sigma_{\mathrm{II}})2\sigma_{\mathrm{II}} n_2^2$$
$$+ (3b\overline{\sigma} + c\sigma_{\mathrm{III}})2\sigma_{\mathrm{III}} n_3^2. \tag{4.66}$$

The latter shows that the anisotropic part of the energy $\mathcal{E}^{(\mathrm{ex})}$ depends upon the TI axis orientation through the three parameters n_1^2, n_2^2 and n_3^2, which satisfy $n_1^2 + n_2^2 + n_3^2 = 1$. Since each of n_1^2, n_2^2 and n_3^2 must be non-negative, the permissible set is the equilateral triangular area A of the plane $n_1^2 + n_2^2 + n_3^2 - 1 = 0$ bounded by the lines $L_1 : n_2^2 + n_3^2 = 1$, $L_2 : n_3^2 + n_1^2 = 1$ and $L_3 : n_1^2 + n_2^2 = 1$.

Consider first the possibility that the optimal orientation lies on one of the lines L_i, $i = 1, 2, 3$. Thus, along L_3, a simple calculation using $n_3^2 = 0$ shows that

$$\mathcal{E}^{(\mathrm{ex})} = a(\sigma_{\mathrm{II}} - \sigma_{\mathrm{I}})^2 \left(n_1^2 - N_1\right)^2 + 2\sigma_{\mathrm{II}}\left(3b\overline{\sigma} + c\sigma_{\mathrm{II}}\right) - a(\sigma_{\mathrm{II}} - \sigma_{\mathrm{I}})^2 N_1^2 \quad \text{on } L_3, \tag{4.67}$$

where

$$N_1 \equiv \frac{a\sigma_{\mathrm{II}} + c(\sigma_{\mathrm{I}} + \sigma_{\mathrm{II}}) + 3b\overline{\sigma}}{a(\sigma_{\mathrm{II}} - \sigma_{\mathrm{I}})}. \tag{4.68}$$

Thus, $n_1^2 = N_1$, is a *possible* optimal orientation. It must first be checked whether or not N_1 lies in $(0, 1)$. If this is so, and if $a > 0$, then an energy minimum occurs at the point $n_1^2 = N_1$, $n_2^2 = 1 - N_1$ on L_3. Similarly, a minimum occurs on L_1 at $n_2^2 = N_2$, $n_3^2 = 1 - N_2$ if $N_2 \in (0, 1)$ and $a > 0$, and on L_2 at $n_3^2 = N_3$, $n_1^2 = 1 - N_3$ if $N_3 \in (0, 1)$ and $a > 0$, where

$$N_2 = \frac{a\sigma_{\mathrm{III}} + c(\sigma_{\mathrm{II}} + \sigma_{\mathrm{III}}) + 3b\overline{\sigma}}{a(\sigma_{\mathrm{III}} - \sigma_{\mathrm{II}})}, \quad N_3 = \frac{a\sigma_{\mathrm{I}} + c(\sigma_{\mathrm{III}} + \sigma_{\mathrm{I}}) + 3b\overline{\sigma}}{a(\sigma_{\mathrm{I}} - \sigma_{\mathrm{III}})}. \tag{4.69}$$

Now consider the possibility of the minimum occurring in the interior of A. Substituting $n_3^2 = 1 - n_1^2 - n_2^2$ into (4.66) and setting the partial derivatives with respect to n_1^2 and n_2^2 to zero, yields a pair of simultaneous conditions:

$$\left(\sigma_{\mathrm{I}} - \sigma_{\mathrm{III}}\right) \left[a\left(\sigma_{\mathrm{I}} n_1^2 + \sigma_{\mathrm{II}} n_2^2 + \sigma_{\mathrm{III}} n_3^2\right) + 3b\overline{\sigma} + c(\sigma_{\mathrm{I}} + \sigma_{\mathrm{III}})\right] = 0, \tag{4.70}$$
$$\left(\sigma_{\mathrm{II}} - \sigma_{\mathrm{III}}\right) \left[a\left(\sigma_{\mathrm{I}} n_1^2 + \sigma_{\mathrm{II}} n_2^2 + \sigma_{\mathrm{III}} n_3^2\right) + 3b\overline{\sigma} + c(\sigma_{\mathrm{II}} + \sigma_{\mathrm{III}})\right] = 0. \tag{4.71}$$

These cannot be satisfied in general if the three principal stresses are distinct. We therefore conclude that *the optimal* **n** *will lie inside A if and only if the stress is biaxial*. For instance, if $\sigma_{\rm II}$ and $\sigma_{\rm III}$ are equal, then (4.70) combined with $n_3^2 = 1 - n_1^2 - n_2^2$ imply that $\mathcal{E}^{(\rm ex)}$ of (4.66) can be expressed as a function of n_1^2 alone, and the expression is identical in form to that given in (4.67). Thus, the existence of a minimum inside A requires biaxiality ($\sigma_{\rm II} = \sigma_{\rm III}$) and that $0 < N_1 < 1$. The associated optimal direction is not unique, but is defined by the cone $n_1^2 = N_1$, $n_2^2 + n_3^2 = 1 - N_1$ (note that $N_3 = 1 - N_1$ when $\sigma_{\rm II} = \sigma_{\rm III}$). Again, (4.67) indicates that the optimal orientation corresponds to a minimum (maximum) in energy if $a > 0$ ($a < 0$). Thus, the sign of the elastic compliance a is crucial in determining whether the stationary point is a minimum or a maximum.

These conclusions may also be confirmed by the coaxiality condition for the stress and strain. Thus, for arbitrary orientation,

$$\begin{aligned}
\varepsilon_{23} &= n_2 n_3\big[a\big(\sigma_{\rm I} n_1^2 + \sigma_{\rm II} n_2^2 + \sigma_{\rm III} n_3^2\big) + 3b\overline{\sigma} + c\big(\sigma_{\rm II} + \sigma_{\rm III}\big)\big],\\
\varepsilon_{31} &= n_3 n_1\big[a\big(\sigma_{\rm I} n_1^2 + \sigma_{\rm II} n_2^2 + \sigma_{\rm III} n_3^2\big) + 3b\overline{\sigma} + c\big(\sigma_{\rm III} + \sigma_{\rm I}\big)\big],\\
\varepsilon_{12} &= n_1 n_2\big[a\big(\sigma_{\rm I} n_1^2 + \sigma_{\rm II} n_2^2 + \sigma_{\rm III} n_3^2\big) + 3b\overline{\sigma} + c\big(\sigma_{\rm I} + \sigma_{\rm II}\big)\big].
\end{aligned} \tag{4.72}$$

The requirement that these simultaneously vanish is identical to the above conditions for the existence of the minimum inside A or along its perimeter.

In summary, $a > 0$ is a necessary condition that an energy minimum occurs at points inside A or along the lines L_j, $j = 1, 2, 3$. A minimum is achieved if and only if one or more of N_1, N_2 or N_3 lies in $(0, 1)$. The minimum occurs on the associated bounding line L_j or on a cone of directions for biaxial states of stress. Otherwise, the global energy minimum corresponds to one of the vertices of A, that is, at $n_1^2 = 1$ or $n_2^2 = 1$ or $n_3^2 = 1$. In this default case the TI axis of symmetry is aligned with one of the stress axes. These findings are in agreement with those of Rovati and Taliercio (**9**), who stated the condition as follows. At least one of the principal axes of stress must lie in a plane of transverse isotropy, or alternatively, the TI axis must lie in a plane defined by a pair of principal axes of stress.

4.4 *Tetragonal symmetry*

The moduli have the same general form as in (4.61), except that there is no relation between $S_{66}^{(0)}$, $S_{11}^{(0)}$ and $S_{12}^{(0)}$. In this sense, tetragonal symmetry is the same as TI but with one additional elastic constant. The isotropic moduli are given by (4.62), and the anisotropic part of the compliance is

$$\begin{aligned}
s_{ijkl}^{(\rm an)} &= a' n_i n_j n_k n_l + b'(\delta_{ij} n_k n_l + \delta_{kl} n_i n_j) + \frac{c'}{2}(\delta_{ik} n_j n_l + \delta_{il} n_j n_k + \delta_{jk} n_i n_l + \delta_{jl} n_i n_k)\\
&\quad + d(p_i p_j - q_i q_j)(p_k p_l - q_k q_l) - \frac{1}{3}(a' + 6b' + 2c')J_{ijkl} - \frac{2}{15}(a' + 5c' + 3d)K_{ijkl}.
\end{aligned}$$

The additional fourth-order tensor as compared to TI is $(p_i p_j - q_i q_j)(p_k p_l - q_k q_l)$, where $\{\mathbf{n}, \mathbf{p}, \mathbf{q}\}$ form an orthonormal triad. The elastic constants a', b', c' and d are

$$\begin{aligned}
a' &= \frac{1}{2}S_{11}^{(0)} + \frac{1}{2}S_{12}^{(0)} + S_{33}^{(0)} + S_{66}^{(0)} - 2S_{13}^{(0)} - 4S_{44}^{(0)},\\
b' &= S_{13}^{(0)} - S_{12}^{(0)} - \frac{1}{2}\big(S_{11}^{(0)} - S_{12}^{(0)}\big) + S_{66}^{(0)},\\
c' &= 2S_{44}^{(0)} - 2S_{66}^{(0)}, \quad d = \frac{1}{2}\big(S_{11}^{(0)} - S_{12}^{(0)}\big) - S_{66}^{(0)}.
\end{aligned} \tag{4.73}$$

Compare with the TI constants a, b, c of (4.64),

$$a' = a - d, \quad b' = b - d, \quad c' = c. \tag{4.74}$$

The strain energy of the tetragonal material can be split into a component similar in form to that for a TI material, and an additional term proportional to the constant d. The minimization of the TI part of the energy is as before (with a', b', c' instead of a, b, c), and depends upon the orientation of $\mathbf{n}$ but not $\mathbf{p}$ and $\mathbf{q}$. The additional energy term depends on the deviatoric part of the stress and on these directions,

$$\mathcal{E}^{\text{tet}} = d\left[(p_i p_j - q_i q_j)\sigma'_{ij}\right]^2 - \frac{2}{5}\, d\sigma'_{ij}\sigma'_{ij}, \tag{4.75}$$

or, in terms of the principal stresses,

$$\mathcal{E}^{\text{tet}} = d\left(\sigma'_{\text{I}}\Delta'_1 + \sigma'_{\text{II}}\Delta'_2 + \sigma'_3\Delta'_{\text{III}}\right)^2 - \frac{2}{5}\, d\sigma'_{ij}\sigma'_{ij}\,, \tag{4.76}$$

where $\Delta'_i = p_i^2 - q_i^2$ (no sum). The final term in (4.76) is independent of $\{\mathbf{n}, \mathbf{p}, \mathbf{q}\}$, and it is only necessary to consider the quantity

$$\mathcal{E}' = d\ f^2, \quad \text{where } f = \sigma'_{\text{I}}\Delta'_1 + \sigma'_{\text{II}}\Delta'_2 + \sigma'_3\Delta'_{\text{III}}. \tag{4.77}$$

The orientation dependence is captured by the quantity f.

It is now demonstrated that for any given $\mathbf{n}$, there is at least one set of $\mathbf{p}, \mathbf{q}$ orthogonal to $\mathbf{n}$ which make $\mathcal{E}'$ vanish. Let $\mathbf{p}^{(0)}, \mathbf{q}^{(0)}$ be an arbitrary pair of unit vectors such that $\{\mathbf{n}, \mathbf{p}^{(0)}, \mathbf{q}^{(0)}\}$ form an orthonormal triad; then every possible set $\{\mathbf{n}, \mathbf{p}, \mathbf{q}\}$ is defined by the pair $\mathbf{p}, \mathbf{q}$ obtained by rotation about $\mathbf{n}$ by angle ϕ:

$$\mathbf{p}(\phi) = \cos\phi\, \mathbf{p}^{(0)} - \sin\phi\, \mathbf{q}^{(0)}, \quad \mathbf{q}(\phi) = \sin\phi\, \mathbf{p}^{(0)} + \cos\phi\, \mathbf{q}^{(0)}. \tag{4.78}$$

It may then be readily verified that

$$\Delta'_i(\phi) = \Delta'_i(0)\ \cos 2\phi - \Delta'_i(\pi/4)\ \sin 2\phi, \quad i = 1, 2, 3. \tag{4.79}$$

Equation (4.79) implies that

$$\mathcal{E}'(\phi) = d\left[f(0)\ \cos 2\phi - f(\pi/4)\ \sin 2\phi\right]^2, \tag{4.80}$$

and hence

$$\mathcal{E}'(\phi^*) = 0, \quad \text{where } \tan 2\phi^* = f(0)/f(\pi/4). \tag{4.81}$$

Thus, if $d > 0$, the situation for tetragonal symmetry is a simple addition to the TI situation. First find $\mathbf{n}$ which minimizes the TI part of the energy. Then, select the pair $\mathbf{p}, \mathbf{q}$ such that they satisfy (4.81). The minimum energy is then exactly that achieved by the TI part of the moduli (although it depends upon a', b', c' rather than a, b and c).

If $d < 0$ then the situation is more complicated, and the sequential minimization of first the TI energy and then the additional energy $\mathcal{E}'$ does not work, although these do define stationary points for the strain energy. The d-term must be taken into account when optimizing with respect to $\mathbf{n}$, and a more complicated minimization problem is involved.

Tetragonal symmetry represents a demarcation between the simpler higher material symmetries for which explicit results can be obtained, and the lower material symmetries which require numerical resolution, in general. Exceptions may occur; however, it is useful and instructive to distinguish the cubic, TI and tetragonal symmetries from those of, for example, monoclinic symmetry with 13 independent moduli to consider.

5. Strain deviation angle

5.1 *Definition of the strain deviation angle*

A necessary condition for an energy minimum is that the stress and strain are coaxial. This is always the case in isotropic media, whereas it will be the exception rather than the rule under conditions of general anisotropy and arbitrary stress. According to Euler's theorem (**20**) the transformation from one set of principal axes to the other can be reduced to an axis of rotation $\mathbf{n}$, $|\mathbf{n}| = 1$, and an angle of rotation ϕ. The stress axes have been assumed to coincide with the fixed axes $\mathbf{e}_j$, $j = 1, 2, 3$. Let $\mathbf{e}'_j$ be the orthonormal axes of the strain tensor, then it follows that the rotation matrix is simply the matrix composed of the three unit vectors as columns:

$$\mathbf{Q} = \left[\mathbf{e}'_1\,\mathbf{e}'_2\,\mathbf{e}'_3\right]. \tag{5.1}$$

Let $\mathbf{Q}$ be represented by (2.10); then it follows from the latter that

$$e_{ijk} Q_{jk} = 2\sin\phi\, n_i. \tag{5.2}$$

This provides a formula to determine both the angle ϕ and the axis of rotation $\mathbf{n}$.

The strain deviation angle ϕ is defined as the angle of rotation between the stress and strain axes. This angle is identically zero in isotropic materials for all stress states. In anisotropic materials it depends on both the material constants and the state of stress. However, the above analysis tells us that $\phi = 0$ is a necessary condition for energy minimization. Therefore, the magnitude of ϕ provides, through a single parameter, the degree to which the given state of stress and material orientation is optimal. It does so without requiring any calculation of the energy locally or globally. It requires only that the principal strain axes are determined, and from those ϕ can be immediately computed.

For a given material, stress and strain, the strain deviation angle can be obtained from (5.2). A more explicit method is to use the general identity for integer m:

$$\cos m\phi = \frac{1}{2}\,\mathrm{tr}(\mathbf{Q}^m) - \frac{1}{2}. \tag{5.3}$$

This follows from, for example, (2.10) and (2.11), which imply

$$\mathbf{Q}^m(\mathbf{n}, \phi) = \mathbf{n}\otimes\mathbf{n} + \cos m\phi\,(\mathbf{I} - \mathbf{n}\otimes\mathbf{n}) + \sin m\phi\,\mathbf{P}. \tag{5.4}$$

For instance, $m = 1$ gives the strain deviation angle explicitly in terms of the first invariant of $\mathbf{Q}$:

$$\phi = \cos^{-1}\left[\tfrac{1}{2}(\mathrm{tr}\mathbf{Q} - 1)\right]. \tag{5.5}$$

5.2 *Weak anisotropy*

Let $\varepsilon_j^{(0)}$, $j = 1, 2, 3$, be the principal strains for the isotropic medium, that is, the principal axes of $s^{(\mathrm{is})}_{ijkl}\sigma_{kl}$, where σ_{ij} is given by (2.1) and/or (2.2). In order to determine ϕ we first need to find the principal axes of strain. It is useful to express the strain as

$$\varepsilon_{ij} = s^{(\mathrm{is})}_{ijkl}\sigma_{kl} + \gamma_{ij}, \tag{5.6}$$

where

$$\gamma_{ij} = s^{(\mathrm{an})}_{ijkl}\sigma_{kl} = s^{(\mathrm{an})}_{ij11}\sigma_{\mathrm{I}} + s^{(\mathrm{an})}_{ij22}\sigma_{\mathrm{II}} + s^{(\mathrm{an})}_{ij33}\sigma_{\mathrm{III}}. \tag{5.7}$$

It is assumed that $\boldsymbol{\gamma}$ is small, so that standard perturbation analysis may be used to find the first correction to the directions of principal strain, $\{\mathbf{e}_1', \mathbf{e}_2', \mathbf{e}_3'\}$, which to leading order are coincident with the stress directions:

$$\mathbf{e}_i' = \mathbf{e}_i + \sum_{j \neq i} \left(\varepsilon_i^{(0)} - \varepsilon_j^{(0)}\right)^{-1} \left(\mathbf{e}_i \cdot \boldsymbol{\gamma}\, \mathbf{e}_j\right) \mathbf{e}_j, \quad \text{no sum on } i. \tag{5.8}$$

Let E and ν be the isotropic Young's modulus and Poisson's ratio characterizing $s_{ijkl}^{(\mathrm{is})}$; then (5.8) implies that, to leading order,

$$Q_{ij} = -Q_{ji} \approx \frac{E}{1+\nu} \frac{\gamma_{ij}}{(\sigma_j - \sigma_i)}, \quad i \neq j. \tag{5.9}$$

Hence, the strain deviation angle for weak anisotropy is

$$\phi \approx \sin\phi \approx \frac{E}{1+\nu} \left[\frac{\gamma_{12}^2}{(\sigma_{\mathrm{I}} - \sigma_{\mathrm{II}})^2} + \frac{\gamma_{23}^2}{(\sigma_{\mathrm{II}} - \sigma_{\mathrm{III}})^2} + \frac{\gamma_{31}^2}{(\sigma_{\mathrm{III}} - \sigma_{\mathrm{I}})^2} \right]^{1/2}. \tag{5.10}$$

It is useful to write the stress dependence explicitly by eliminating $\boldsymbol{\gamma}$:

$$\phi \approx \frac{E}{1+\nu} \left[\left(\frac{\sigma_{\mathrm{I}} s_{14}^{(\mathrm{an})} + \sigma_{\mathrm{II}} s_{24}^{(\mathrm{an})} + \sigma_{\mathrm{III}} s_{34}^{(\mathrm{an})}}{\sigma_{\mathrm{II}} - \sigma_{\mathrm{III}}} \right)^2 + \left(\frac{\sigma_{\mathrm{I}} s_{15}^{(\mathrm{an})} + \sigma_{\mathrm{II}} s_{25}^{(\mathrm{an})} + \sigma_{\mathrm{III}} s_{35}^{(\mathrm{an})}}{\sigma_{\mathrm{III}} - \sigma_{\mathrm{I}}} \right)^2 \right.$$
$$\left. + \left(\frac{\sigma_{\mathrm{I}} s_{16}^{(\mathrm{an})} + \sigma_{\mathrm{II}} s_{26}^{(\mathrm{an})} + \sigma_{\mathrm{III}} s_{36}^{(\mathrm{an})}}{\sigma_{\mathrm{I}} - \sigma_{\mathrm{II}}} \right)^2 \right]^{1/2}. \tag{5.11}$$

This shows that the strain deviation angle depends upon the same nine moduli that appear in the matrix $\mathbf{E}$ of (3.10).

The above formula breaks down for biaxial stress. In this case the choice of fixed axes is arbitrary since any orthogonal pair in the plane spanned by the equal principal stresses are valid. However, the choice can be made *a posteriori* such that the term that would otherwise be singular is zero. For instance, if $\sigma_{\mathrm{I}} = \sigma_{\mathrm{II}}$, then the axes $\mathbf{e}_1$ and $\mathbf{e}_2$ can be selected such that $\gamma_{12} = 0$.

6. Conclusions

The six-dimensional notation of Mehrabadi *et al.* (**15**) is well suited to the problem of finding optimal orientations of anisotropic solids. It leads quite naturally to the main results of this paper, which we recapitulate.

RESULT 1 The energy $\mathcal{E}$ is stationary if and only if the stress and strain are coaxial.

RESULT 1a A necessary (but not sufficient) condition for this to hold is that $\det \mathbf{E} = 0$, where $\mathbf{E}$ is defined in (3.10)

RESULT 2 The energy $\mathcal{E}$ is a local minimum if the stress and strain are coaxial and the symmetric matrix $\mathbf{G}$ of (3.20) is positive definite.

Result 2 provides for the first time an explicit set of conditions that must be satisfied if the stationary condition is a minimum or a maximum.

Specific results are given for materials of cubic, transversely isotropic and tetragonal symmetries. In each case the existence of a minimum or maximum depends on the sign of a single elastic constant. For cubic symmetry we have several new findings. For instance, (4.45) to (4.47) provide a two-parameter set of stress states which minimize or maximize the strain energy if a material of cubic symmetry is rotated about an arbitrary axis **n** by an angle ϕ (subject to the constraint (4.48)). Alternatively, (4.52) and (4.53) provide a means to find the optimal orientation for a given state of stress. In particular, the rotation of the material axes depends only upon the deviatoric stress. This demonstrates that the stationary (minimum or maximum) value of energy can always be achieved for cubic materials. Furthermore, it shows that the optimal orientation of a solid with cubic material symmetry is not normally aligned with the symmetry directions.

The remainder of the new results concern the optimal orientation of TI and tetragonal materials, and are in general agreement with results of Rovati and Taliercio (**9**) obtained by a different procedure. However, the results obtained here are more direct and provide considerable insight into the nature of the optimal states for these material symmetries. In particular, the problem for tetragonal symmetry is very similar to that for TI, with an additional energy term that can be simply minimized or maximized (depending on the sign of the constant d of (4.73)).

Finally, we have defined and introduced the strain deviation angle. This angle is inherently anisotropic, and directly related to the problem of energy minimization since the angle defines the degree to which a state of stress or strain is not optimal. Future work will explore other consequences of this new concept.

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APPENDIX

Two-dimensional elasticity

Optimal orientation for two-dimensional elastic anisotropy is an important special case of the general problem. It was recently considered by Gea and Luo (**12**), and is reconsidered here in the context of the present theory. We will see that some of the features Gea and Luo obtained transfer to the three-dimensional problem: in particular, the dependence of the minimization upon a single elastic constant.

The two-dimensional strain–energy function is

$$\mathcal{E}(\theta) = S_{11}\sigma_{\mathrm{I}}^2 + S_{22}\sigma_{\mathrm{II}}^2 + 2S_{12}\sigma_{\mathrm{I}}\sigma_{\mathrm{II}}\,, \tag{A.1}$$

where S_{11}, S_{22} and S_{12} depend upon the angle θ by which the material is rotated relative to the fixed $\mathbf{e}_3$ axis. Consider an orthotropic material with compliance elements $S_{11}^{(0)}$, $S_{22}^{(0)}$, $S_{12}^{(0)}$, $S_{66}^{(0)}$ in the unrotated (fixed) axes. Using the standard relations (**21**) for the transformation of the moduli, it can be shown that

$$\mathcal{E}(\theta) = \frac{1}{4}\, d_0(\sigma_{\mathrm{II}} - \sigma_{\mathrm{I}})^2(\cos 2\theta - \Lambda)^2 + b_0, \tag{A.2}$$

where $\Lambda = (c_0/d_0)(\sigma_{\mathrm{II}} + \sigma_{\mathrm{I}})/(\sigma_{\mathrm{II}} - \sigma_{\mathrm{I}})$ is a combination of stress and moduli, c_0 and d_0 are moduli,

$$c_0 = S_{11}^{(0)} - S_{22}^{(0)}, \quad d_0 = S_{11}^{(0)} + S_{22}^{(0)} - 2S_{12}^{(0)} - 4S_{66}^{(0)}, \tag{A.3}$$

and $b_0 = (\sigma_{\mathrm{II}} - \sigma_{\mathrm{I}})^2\, S_{66}^{(0)} + \frac{1}{4}(\sigma_{\mathrm{II}} + \sigma_{\mathrm{I}})^2 \left(S_{11}^{(0)} + S_{22}^{(0)} + 2S_{12}^{(0)} - c_0^2/d_0\right)$ is a constant.

It can easily be seen that the energy $\mathcal{E}$ of (A.2) is stationary with respect to θ when

$$\cos 2\theta = 1, \text{ and } \cos 2\theta = -1 \Leftrightarrow \theta = 0, \text{ and } \theta = \pi/2, \tag{A.4}$$

respectively. Which of these yields the smaller value for $\mathcal{E}$ depends upon the sign of $d_0\Lambda$ or, equivalently, the sign of $(\sigma_{\mathrm{II}}^2 - \sigma_{\mathrm{I}}^2)c_0$. Specifically, the minimum is at $\cos 2\theta = \mathrm{sgn}[(\sigma_{\mathrm{II}}^2 - \sigma_{\mathrm{I}}^2)c_0]$. A third stationary value is possible if $-1 < \Lambda < 1$, and occurs at

$$\cos 2\theta = \Lambda, \Leftrightarrow \theta = \pm\theta^*, \tag{A.5}$$

where $\theta^* = \frac{1}{2}\cos^{-1}\Lambda$. If this stationary point occurs, it follows from explicit evaluation that it corresponds to a global minimum or maximum of the energy. Thus,

$$\mathcal{E}(0) = b_0 + d_0(\sigma_{\mathrm{II}} - \sigma_{\mathrm{I}})^2 \sin^4\theta^*, \quad \mathcal{E}(\pi/2) = b_0 + d_0(\sigma_{\mathrm{II}} - \sigma_{\mathrm{I}})^2 \cos^4\theta^*, \quad \mathcal{E}(\theta^*) = b_0. \tag{A.6}$$

It is clear that $\theta = \pm\theta^*$ is a repeated global minimum (maximum) if $d_0 > 0$ ($d_0 < 0$). This is the fundamental result of Gea and Luo (**12**) (although their conclusion is slightly different since they do not start with the stress in the principal axes frame): if $-1 < \Lambda < 1$ and $d_0 > 0$ then $\theta = \pm\theta^*$ is a repeated global minimum of $\mathcal{E}(\theta)$. Otherwise, the minimum occurs when $\cos 2\theta = \mathrm{sgn}[(\sigma_{\mathrm{II}}^2 - \sigma_{\mathrm{I}}^2)c_0]$.

The results of Gea and Luo are now reconsidered within the context of the general theory applied to two dimensions. Based on the general theory for three dimensions, the two-dimensional condition for a stationary orientation is $\varepsilon_{12} = 0$ or, in terms of the stress, assuming for simplicity that $\sigma_{\mathrm{III}} = 0$,

$$S_{16}\sigma_{\mathrm{I}} + S_{26}\sigma_{\mathrm{II}} = 0. \tag{A.7}$$

The latter is consistent with the general formulation, (3.8), under the assumption that σ_{I} and σ_{II} are distinct (if they are not distinct, then the stress-based energy function is constant for all material orientations). The additional condition that the stationary orientation is a local minimum follows from

$$\left.\frac{d^2\mathcal{E}(\theta)}{d\theta^2}\right|_{\theta=0} = 4F_{33}, \tag{A.8}$$

as $F_{33} = 2(\sigma_{\mathrm{II}} - \sigma_{\mathrm{I}})^2 G_{33} > 0$. The exact form of G_{33} follows from (3.19) with $\sigma_{\mathrm{III}} = 0$ as

$$G_{33} = S_{66} + (\sigma_{\mathrm{II}} - \sigma_{\mathrm{I}})^{-1}\,[(S_{11} - S_{12})\sigma_{\mathrm{I}} + (S_{21} - S_{22})\sigma_{\mathrm{II}}]/2. \tag{A.9}$$

Rearrangement gives

$$G_{33} = (\sigma_{\mathrm{II}} - \sigma_{\mathrm{I}})^{-1}\,[(\sigma_{\mathrm{I}} + \sigma_{\mathrm{II}})c + (\sigma_{\mathrm{I}} - \sigma_{\mathrm{II}})d]/4, \tag{A.10}$$

where c and d are

$$c = S_{11} - S_{22}, \qquad d = S_{11} + S_{22} - 2S_{12} - 4S_{66}. \tag{A.11}$$

The specific case of an orthotropic material is considered next. It may be shown by use of standard relations (**21**) that the combinations of moduli in (A.11) transform according to $c(\theta) = c_0 \cos 2\theta$, $d(\theta) = d_0 \cos 4\theta$, where $c_0 = c(0)$ and $d_0 = d(0)$ are the same moduli defined in (A.3). Also,

$$S_{16} = -\frac{1}{4}\left(c_0 + d_0\cos 2\theta\right)\,\sin 2\theta, \quad S_{26} = -\frac{1}{4}\left(c_0 - d_0\cos 2\theta\right)\,\sin 2\theta. \tag{A.12}$$

Hence, $\varepsilon_{12} = -\frac{1}{4}\sin 2\theta\,\left[(\sigma_{\mathrm{I}} + \sigma_{\mathrm{II}})c_0 + (\sigma_{\mathrm{I}} - \sigma_{\mathrm{II}})d_0\cos 2\theta\right]$. The strain ε_{12} vanishes if $\sin 2\theta = 0$ or $\cos 2\theta = \Lambda$. Thus, the stationary points are $\theta = 0,\ \pi/2$ and $\pm\theta^*$ where $\cos 2\theta^* = \Lambda$, in agreement with (**12**).

Using the same notation, (A.10) becomes $G_{33}(\theta) = \frac{1}{4}d_0(\Lambda\cos 2\theta - \cos 4\theta)$. In particular, if $-1 < \Lambda < 1$, then $G_{33}(\theta^*) = \frac{1}{4}d_0\sin^2 2\theta^*$. This implies that $\theta = \pm\theta^*$ is a local minimum of $\mathcal{E}$ if and only if d_0 is positive. The general analysis for three-dimensional optimal orientation does not provide an explicit statement about global minima. In order to show that it is a global maximum one must compare the value of $\mathcal{E}$ at $\theta = \pm\theta^*$ with its value at the other local minimum, as done in (A.6).