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The Elastic Tensor of Given Symmetry Nearest to an Anisotropic Elastic Tensor

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Given an arbitrary tensor in an n-dimensional Euclidean space, it is required to find its 'nearest' tensor of some preassigned symmetry, *i.e.* the tensor of this symmetry which has the minimum invariant 'distance' from the given tensor. General theorems are given concerning the construction and properties of these nearest tensors. The theorems are applied, in the case of elastic tensors, for the construction of the nearest isotropic and cubic tensors to a given anisotropic elastic tensor, and the nearest hexagonal polar tensor to a cubic elastic tensor.

1. Introduction

An investigation of the elastic properties of an anisotropic body can sometimes be aided by a knowledge of the corresponding properties of an isotropic elastic body having the same shape and proximal stress-strain relations. For example, the frequency spectrum of the normal vibrations of an anisotropic body which is nearly isotropic may be determined by the method of perturbations, starting from the known spectrum and modes of vibration of a proximal isotropic material. For such a calculation, it is desirable to begin with the isotropic material which, in some sense, is 'nearest' to the given anisotropic material. A natural definition and a simple method for constructing the isotropic elastic tensor nearest to a given elastic tensor is given in this paper.

The problem of constructing the isotropic elastic tensor nearest to a given elastic tensor of lower symmetry can be generalized in a number of directions. First of all, the same methods we have devised for solving this problem can be used to determine the elastic tensor of *any* preassigned symmetry which is nearest to a given elastic tensor. Secondly, the methods and general theorems we have established are not restricted to tensors of the particular rank and symmetry of elastic tensors. Moreover, the general invariance theorems, which, in view of the intended applications, have been proved for finite dimensional spaces only, can easily be extended to infinite dimensional spaces, and hence may find application in analysis.

General theorems concerning tensors of any rank in an n-dimensional Euclidean space are given in Section 2. Section 3 contains the construction of the nearest isotropic tensor to a given anisotropic elastic tensor, and Section 4 a similar construction of the nearest cubic tensor. Finally, in Section 5, we discuss how the present theorems can be applied to other symmetry groups of crystals and give the construction of the nearest hexagonal polar tensor to a cubic tensor.

2. The general theory

We shall assume the reader is familiar with the definition and algebra of tensors with finite dimensional carrier spaces. For completeness, and to introduce our terminology and notations, we preface this section with a brief listing of the relevant definitions.

Let E^n denote an n-dimensional Euclidean space with real positive definite inner product $(\mathbf{a}, \mathbf{b})$; $\mathbf{a}, \mathbf{b} \in E^n$. A real linear transformation $\mathbf{O}$ of $E^n \to E^n$ that preserves all inner products is an *orthogonal transformation*. Thus, $\mathbf{O}$ is orthogonal if and only if

$$(\mathbf{Oa}, \mathbf{Ob}) = (\mathbf{a}, \mathbf{b}) \tag{2·1}$$

for every pair of vectors $\mathbf{a}$ and $\mathbf{b}$. The *adjoint* $\mathbf{A}^\dagger$ of any linear transformation $\mathbf{A}$ of E^n is defined by the condition

$$(\mathbf{A}^\dagger\mathbf{a}, \mathbf{b}) = (\mathbf{a}, \mathbf{Ab}) \, . \tag{2·2}$$

With respect to an orthonormal system of basis vectors in E^n, an orthogonal transformation is represented by an *orthogonal matrix* O_{ij} and

$$O_{ij}O_{kj} = \delta_{ik} \tag{2·3}$$

where δ_{ik} are the components of the unit matrix and we use the summation convention for repeated indices. In matrix notation, (2·3) reads $\mathbf{O}.\mathbf{O}^T = \mathbf{I}$, where $\mathbf{O}^T$ denotes the transpose of the matrix $\mathbf{O}$, and $\mathbf{I}$ denotes the unit matrix. Thus, the matrix of an orthogonal transformation with respect to an *orthonormal* basis satisfies the condition $\mathbf{O}^T = \mathbf{O}^{-1}$. More generally, however, from (2·1) and the definition of the adjoint we have, with respect to any basis, $\mathbf{O}^\dagger = \mathbf{O}^{-1}$, a property we shall need in the sequel.

The *components of the metric tensor* with respect to a *basis* $\mathbf{e}_i$ of E^n are defined by

$$g_{ij} \equiv (\mathbf{e}_i, \mathbf{e}_j) \, . \tag{2·4}$$

As is customary in geometry and physics, we shall not distinguish between covariant, contravariant, and mixed tensors having the same rank and carrier

space E^n. The covariant, contravariant, and mixed components of a tensor $\mathbf{T}$ are related to one another by the familiar process of raising and lowering the indices of their components. For example, if $\mathbf{T}$ is a given tensor with contravariant components T^{ij} relative to a basis $\mathbf{e}_i$, then $\mathbf{T}=T^{ij}\mathbf{e}_i\otimes\mathbf{e}_j=T^i_j\mathbf{e}_i\otimes\mathbf{e}^j=T_{ij}\mathbf{e}^i\otimes\mathbf{e}^j$, where $T^i_j=g_{jk}T^{ik}$, $T_{ij}=g_{ik}g_{jl}T^{kl}$ and $\mathbf{e}^i$ denotes the basis of the conjugate space E_n of E^n which is reciprocal to the basis $\mathbf{e}^i$ of E^n, *i.e.*, $\mathbf{e}^i(\mathbf{e}_j)=\delta^i_j$.

Let E^{n^k} denote the n^k-dimensional space of tensors of rank k with carrier space E^n, and let $\boldsymbol{G}$ denote a group of orthogonal transformations of E^n. Each linear transformation $\mathbf{G}\in\boldsymbol{G}$ of E^n induces a corresponding linear transformation $\mathbf{G}:E^{n^k}\to E^{n^k}$, given by the usual tensor law. An *invariant tensor* of the group $\boldsymbol{G}$ is any tensor $\mathbf{T}$ such that $\mathbf{G}.\mathbf{T}=\mathbf{T}$ for every $\mathbf{G}\in\boldsymbol{G}$. Since every $\mathbf{G}$ is linear, if $\mathbf{T}$ and $\mathbf{U}$ are invariant tensors, then so also is $\lambda\mathbf{T}+\eta\mathbf{U}$, where λ and η are arbitrary scalars. Thus, the set of all invariant tensors of a group $\boldsymbol{G}$ having given rank and carrier space E^n form a subspace of E^{n^k} for an appropriate value of k. Now each E^{n^k} is finite-dimensional with a positive definite inner product defined by

$$(\mathbf{T},\mathbf{U})\equiv T^{i_1i_2\ldots i_k}U_{i_1i_2\ldots i_k}\equiv g_{i_1j_1}g_{i_2j_2}\ldots g_{i_kj_k}T^{i_1i_2\ldots i_k}U^{j_1j_2\ldots j_k}. \quad (2\cdot5)$$

It is always possible to construct an orthonormal basis of tensors in E^{n^k} such that the first N members span the subspace of invariant tensors of $\boldsymbol{G}$ in E^{n^k} while the remaining n^k-N members span the complement. Let $\mathbf{A}_p$, $p=1,2,\ldots,N$ and $\mathbf{B}_q$, $q=1,2,\ldots,n^k-N$ denote the elements of such a basis. An arbitrary tensor $\mathbf{T}\in E^{n^k}$ can then be expressed in the form

$$\mathbf{T}=\sum_{p=1}^{N}(\mathbf{A}_p,\mathbf{T})\mathbf{A}_p+\sum_{q=1}^{n^k-N}(\mathbf{B}_q,\mathbf{T})\mathbf{B}_q={}_G\mathbf{T}+\mathbf{T}^* \quad (2\cdot6)$$

where ${}_G\mathbf{T}$ denotes the sum of the first N terms in (2·6) and $\mathbf{T}^*$ denotes the sum of the last n^k-N terms. Now ${}_G\mathbf{T}$ is an invariant tensor of the group $\boldsymbol{G}$ as is every element $\mathbf{A}_p$. Also, ${}_G\mathbf{T}$ is the normal projection of $\mathbf{T}$ into the subspace of invariant tensors of $\boldsymbol{G}$. We call $\mathbf{T}^*$ the *residue of* $\mathbf{T}$ *relative to the group* $\boldsymbol{G}$ and we call ${}_G\mathbf{T}$ the *tensor of symmetry* $\boldsymbol{G}$ *nearest to the tensor* $\mathbf{T}$. It is nearest in the sense that it is the element of the subspace of invariant tensors of $\boldsymbol{G}$ which minimizes the 'distance' $D^2=(\mathbf{T}-{}_G\mathbf{T},\mathbf{T}-{}_G\mathbf{T})$.

In general, suppose one is given a particular tensor $\mathbf{C}$ of rank k. One easily sees that the set of all orthogonal transformations $\mathbf{O}$ such that $\overline{\mathbf{C}}=\mathbf{C}$, where $\overline{\mathbf{C}}\equiv\mathbf{O}.\mathbf{C}$, form a group, ${}_C\boldsymbol{G}$ say. We call ${}_C\boldsymbol{G}$ the invariance group, or *symmetry group*, of the tensor $\mathbf{C}$. The orthogonal group, for example, is the symmetry group of the metric tensor $\mathbf{g}$.

Consider next an arbitrary group of orthogonal transformations, $\boldsymbol{G}$, finite or infinite, for which the process of group integration can be defined.‡ Let the symbol $\int_{\boldsymbol{G}}$ denote *averaging* over the group, *i.e.* summation and/or integration divided by the 'volume' of the group. Let $\mathbf{C}$ be an arbitrary tensor of rank k and consider the average of the transform of $\mathbf{C}$ over the group

$$\hat{\mathbf{C}}=\int_{\mathbf{O}\in\boldsymbol{G}}\mathbf{O}.\mathbf{C}. \quad (2\cdot7)$$

The average tensor $\hat{\mathbf{C}}$ is always an invariant tensor of the group $\boldsymbol{G}$. Hence, averaging over the group defines a certain linear mapping of the whole space E^{n^k} into the subspace of invariant tensors of $\boldsymbol{G}$. Normal projection described above provides a similar mapping. Theorem (2·1), which follows, states that these mappings are one and the same mapping.

Theorem (2·1): *The tensor* ${}_G\mathbf{C}$ *of symmetry* $\boldsymbol{G}$ *nearest to a given tensor* $\mathbf{C}$ *is equal to the average of the transform of* $\mathbf{C}$ *over the group* $\boldsymbol{G}$ *of orthogonal transformations.*

Proof: It suffices to show that the components $(\mathbf{A}_p,\hat{\mathbf{C}})$ and $(\mathbf{A}_p,\mathbf{C})$ are equal respectively, where $\mathbf{A}_p$ is an arbitrary orthonormal basis for the subspace of invariant tensors of $\boldsymbol{G}$ in E^{n^k}. We have

$$(\mathbf{A}_p,\hat{\mathbf{C}})=\int_{\boldsymbol{G}}(\mathbf{A}_p,\mathbf{O}(\mathbf{C}))=\int_{\boldsymbol{G}}(\mathbf{O}^\dagger(\mathbf{A}_p),\mathbf{C}). \quad (2\cdot8)$$

But, since every $\mathbf{O}\in\boldsymbol{G}$ is orthogonal, $\mathbf{O}^\dagger=\mathbf{O}^{-1}$, and since $\boldsymbol{G}$ is a group, it contains $\mathbf{O}^{-1}$ if it contains $\mathbf{O}$. But $\mathbf{A}_p$ is, by hypothesis, an invariant tensor of $\boldsymbol{G}$ so that $\mathbf{O}^{-1}(\mathbf{A}_p)=\mathbf{O}^\dagger(\mathbf{A}_p)=\mathbf{A}_p$. Thus (2·8) becomes

$$(\mathbf{A}_p,\hat{\mathbf{C}})=\int_G(\mathbf{A}_p,\mathbf{C})=(\mathbf{A}_p,\mathbf{C}) \quad (2\cdot9)$$

which proves the theorem.§

Let $\mathbf{C}$ be a tensor of even rank $2r$. We say that $\mathbf{C}$ is *positive definite* if

$$(\mathbf{e},\mathbf{Ce})\equiv C_{i_1i_2\ldots i_rj_1j_2\ldots j_r}e^{i_1i_2\ldots i_r}e^{j_1j_2\ldots j_r}>0 \quad (2\cdot10)$$

for every tensor $\mathbf{e}\neq0$.

Theorem (2·2): *The average of the transform of a positive definite tensor over any group of transformations is positive definite.*

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‡ For finite groups, integration over the group reduces to summation and is always possible. For infinite groups, the theory is given by Weyl (1946).

§ It may be pointed out that nothing in the proof depends in an essential way upon the finite dimension of E^n so that the result established here for finite dimensional spaces E^n can also be established for E^n replaced by a Hilbert space H. Also, the real metric assumed here may be replaced by a positive definite Hermitian form and the orthogonal group replaced by the unitary group. However, our applications do not require these possible generalizations.

The proof is trivial. We have

$$(\mathbf{e}, \mathbf{O}(\mathbf{C})\mathbf{e}) = (\mathbf{O}^{\dagger}(\mathbf{e}), \mathbf{C}\mathbf{O}^{\dagger}(\mathbf{e})) . \tag{2·11}$$

Hence

$$(\mathbf{e}, \hat{\mathbf{C}}\mathbf{e}) = \int_{\boldsymbol{G}} (\mathbf{O}^{\dagger}(\mathbf{e}), \mathbf{C}\mathbf{O}^{\dagger}(\mathbf{e})) > 0$$

for every $\mathbf{e} \neq 0$ provided $\mathbf{C}$ is positive definite.

As a corollary of theorems (2·1) and (2·2) we have

Corollary (2·1): *The nearest tensor of symmetry* $\boldsymbol{G}$ *to a positive definite tensor is always positive definite.*

3. The isotropic elastic tensor nearest to an elastic tensor of arbitrary symmetry

In classical linear elasticity theory the elastic properties of a homogeneous material are completely determined by the stress-strain relations which we write in the form

$$t^{ij} = C^{ijkl} e_{kl} \tag{3·1}$$

where $t^{ij} = t^{ji}$ are the components of the stress tensor and $e_{ij} = e_{ji}$ are the components of the tensor measure of infinitesimal strain. Thus, within the linear theory, the material properties are fixed in terms of the *elastic tensor* $\mathbf{C}$. Every elastic tensor satisfies the relations

$$C^{ijkl} = C^{jikl} = C^{ijlk} = C^{klij} \tag{3·2}$$

and is positive definite in the sense of (2·10). We adopt the view that any positive definite tensor $\mathbf{C}$ of rank four satisfying the relations (3·2) defines a possible elastic material.

A tensor invariant of the full orthogonal group is called an *isotropic tensor*. To construct the nearest isotropic tensor to a given elastic tensor $\mathbf{C}$, we can, by theorem (2·1), follow either of two procedures: (1) average $\mathbf{C}$ over the orthogonal group, or (2) construct an orthonormal basis of isotropic tensors of rank four which span the subspace of isotropic tensors having the symmetry (3·2). By theorem (2·2) and corollary (2·1) we are assured that the isotropic tensor nearest to any elastic tensor $\mathbf{C}$ will be positive definite and, therefore, an elastic tensor also. The construction of the nearest isotropic tensor according to the second procedure is the easiest.

Two orthonormal isotropic tensors satisfying the symmetry relations (3·2) can be constructed by taking suitable linear combinations of the two isotropic tensors

$$\begin{aligned} E_{(1)ijkl} &= g_{ij} g_{kl} , \\ E_{(2)ijkl} &= g_{ik} g_{kl} + g_{il} g_{jk} , \end{aligned} \tag{3·3}$$

and it is known that every isotropic tensor of rank four satisfying (3·2) is a linear combination of $\mathbf{E}_{(1)}$ and $\mathbf{E}_{(2)}$. One set of orthonormal isotropic tensors is given by

$$\begin{aligned} \mathbf{A}_1 &= \tfrac{1}{3}\mathbf{E}_1 , \\ \mathbf{A}_2 &= \frac{1}{6\sqrt{5}} (3\mathbf{E}_2 - 2\mathbf{E}_1) . \end{aligned} \tag{3·4}$$

In the Voigt notation for a 6×6 elastic tensor, the tensors $\mathbf{A}_J$, $J = 1, 2$ have components given explicitly by

$$\mathbf{A}_1 = \tfrac{1}{3} \begin{bmatrix} 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix},$$

$$\mathbf{A}_2 = \frac{1}{6\sqrt{5}} \begin{bmatrix} 4 & -2 & -2 & 0 & 0 & 0 \\ -2 & 4 & -2 & 0 & 0 & 0 \\ -2 & -2 & 4 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 3 \end{bmatrix}. \tag{3·5}$$

Any other orthonormal set of isotropic tensors, $\mathbf{B}_J$, is expressible in terms of the $\mathbf{A}_J$ by means of the formula

$$\mathbf{B}_J = b_J^I \mathbf{A}_I , \tag{3·6}$$

where summation from 1 to 2 over repeated capital indices is implied, and b_J^I is a 2×2 orthogonal matrix having the form

$$||b_J^I|| = \begin{bmatrix} \cos\theta & \sin\theta \\ \mp\sin\theta & \pm\cos\theta \end{bmatrix} \tag{3·7}$$

with θ a parameter.

An arbitrary elastic tensor $\mathbf{C}$ may now be expressed as a sum of three components:

$$\mathbf{C} = (\mathbf{C}, \mathbf{A}_1)\mathbf{A}_1 + (\mathbf{C}, \mathbf{A}_2)\mathbf{A}_2 + \mathbf{C}^* \tag{3·8}$$

where the isotropic residue $\mathbf{C}^*$ is the difference between $\mathbf{C}$ and its nearest isotropic tensor which is the sum of the first two terms on the right-hand side of (3·8). We may note that the isotropic tensors $\mathbf{A}_J$ are *not* elastic tensors since each is only positive semi-definite. Moreover, the isotropic residue $\mathbf{C}^*$ is always indefinite or semi-definite. The basis $\mathbf{A}_J$ is distinguished by the property that each element of the basis is positive semi-definite. From the formulae (3·6) and (3·7) it can be easily seen that the elements $\mathbf{B}_J$ of any other orthonormal basis for isotropic tensors of this symmetry consist in one definite (positive or negative definite) element and one indefinite element.

Given an arbitrary elastic matrix in the Voigt notation, the nearest isotropic elastic tensor is particularly easy to compute using the formulae (3·5) and (3·8).

For convenience in computing the inner product $(\mathbf{C}, \mathbf{D})$ when $\mathbf{C}$ and $\mathbf{D}$ are given in the Voigt notation. we give the following formula:

$$(\mathbf{C}, \mathbf{D}) = \text{trace}\,(Q.C.Q.D) \tag{3·9}$$

where, on the right-hand side, C and D are the 6×6 Voigt matrices, a dot denotes matrix multiplication, and

$$Q = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 \end{bmatrix}. \quad (3\cdot 10)$$

4. The nearest cubic tensor

A *cubic elastic tensor* is an elastic tensor whose symmetry group is generated by the permutations of its symmetry axes ($\mathbf{e}_1$, $\mathbf{e}_2$, $\mathbf{e}_3$) and the reflections $\mathbf{e}_i \to -\mathbf{e}_i$. If the coordinate axes are chosen so as to coincide with the symmetry axes of the material, the transformations which leave C_{ijkl} invariant are the transformations $\mathbf{O}$ which permute and reflect the axes of the coordinate system in any fashion.

An arbitrary cubic elastic tensor is expressible in the form

$$\mathbf{C} = \alpha_1\mathbf{A}_1 + \alpha_2\mathbf{A}_2 + \alpha_3\mathbf{A}_3\,, \quad (4\cdot 1)$$

where $\mathbf{A}_J$, $J=1, 2, 3$ is an orthonormal set composed of the isotropic tensors $\mathbf{A}_1$ and $\mathbf{A}_2$ given in (3·5) and a cubic tensor $\mathbf{A}_3$. If the axes of the coordinate system coincide with the axes of the given cubic tensor, then $\mathbf{A}_3$ has components, in the Voigt notation,

$$A_3 = \frac{1}{\sqrt{30}} \begin{bmatrix} -2 & 1 & 1 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 & 0 \\ 1 & 1 & -2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}. \quad (4\cdot 2)$$

An arbitrary elastic tensor $\mathbf{C}$ can be written in the form

$$\begin{aligned} \mathbf{C} &= \sum_{J=1}^{3} (\mathbf{A}_J, \mathbf{C})\mathbf{A}_J + \mathbf{C}^* \quad (4\cdot 3)\\ &= {}_c\mathbf{C} + \mathbf{C}^*, \end{aligned}$$

where $\mathbf{C}^*$ is the *cubic residue* and ${}_c\mathbf{C}$ is the cubic tensor having the symmetry axes of $\mathbf{A}_3$ which is nearest to the given tensor $\mathbf{C}$. By corollary (2·1), ${}_c\mathbf{C}$ is positive definite.

Now the symmetry axes of $\mathbf{A}_3$, which determine the symmetry axes of ${}_c\mathbf{C}$, were chosen in a perfectly arbitrary way. The resolution (4·3) minimizes the length $(\mathbf{C}^*, \mathbf{C}^*)$ of the residue for this particular choice of the symmetry axes of the cubic part. However, in general, there exists another cubic tensor with symmetry axes different from $\mathbf{A}_3$ such that, in a similar resolution of the same tensor $\mathbf{C}$, the residue has smaller length. To determine the direction of the symmetry axes of the cubic tensor for which the residue of a given tensor $\mathbf{C}$ has the smallest length is a more difficult problem. The problem is only partially resolved by the following considerations.

Let $T.A_3$ denote an orthogonal transformation of the particular cubic tensor (4·2). The tensors A_1, A_2, and $T.A_3$ form an orthonormal basis for cubic elastic tensors having the symmetry axes of $\mathbf{T}.\mathbf{A}_3$. With respect to this new basis, an arbitrary elastic tensor $\mathbf{C}$ is decomposed as follows:

$$\mathbf{C} = (\mathbf{C}, \mathbf{A}_1)\mathbf{A}_1 + (\mathbf{C}, \mathbf{A}_2)\mathbf{A}_2 + (\mathbf{C}, \mathbf{T}.\mathbf{A}_3)\mathbf{T}.\mathbf{A}_3 + \mathbf{C}^*(\mathbf{T}) \quad (4\cdot 4)$$

where the residue now depends on $\mathbf{T}$ as indicated. The cubic elastic tensor nearest to $\mathbf{C}$ is now given by the first three terms in (4·4) for that value of $\mathbf{T}$ which minimizes $|\mathbf{C}^*(\mathbf{T})|$.

Suppose that the axes of $\mathbf{A}_3$ coincide with the axes of symmetry of the cubic elastic tensor nearest to $\mathbf{C}$. In this case, the quantity

$$G \equiv (\mathbf{C}, \mathbf{T}.\mathbf{A}_3) \quad (4\cdot 5)$$

will have a stationary value at $\mathbf{T}=\mathbf{I}$, for arbitrary infinitesimal rotations. Let C_{ijkl} be the components of $\mathbf{C}$ in the coordinate system whose axes coincide with the symmetry axes of its nearest cubic elastic tensor, and let A_{ijkl} denote the corresponding components of $\mathbf{A}_3$ given in the Voigt notation by (4·2). An infinitesimal rotation $\mathbf{T}$ has Cartesian components given by

$$T_{ij} = \delta_{ij} + \varepsilon_{ij}, \quad \varepsilon_{ij} = -\varepsilon_{ji}\,. \quad (4\cdot 6)$$

The first variation of the function G is then given by

$$\begin{aligned} \delta G &= \varepsilon_{ip}C_{ijkl}(A_{pjkl} + A_{jpkl} + A_{jlpk} + A_{jlkp})\\ &= 2\varepsilon_{ip}C_{ijkl}(A_{pjkl} + A_{jlkp}) \quad (4\cdot 7) \end{aligned}$$

which must vanish for arbitrary ε_{ij}. Inserting the values of the A_{ijkl} as given by (4·2), we deduce:

Theorem (4·1): *Given the components of an elastic tensor* $\mathbf{C}$ *in a particular coordinate system, a necessary condition that the axes of the coordinate system coincide with the axes of the cubic elastic tensor nearest to* $\mathbf{C}$ *is that the Voigt components of* $\mathbf{C}$ *satisfy the relations*

$$C_{16} = C_{26}, \quad C_{24} = C_{34}, \quad C_{35} = C_{15}\,. \quad (4\cdot 8)$$

We should caution that the relations (4·8) are only necessary, not sufficient, and we have not completely solved the problem of determining the cubic tensor nearest to a given elastic tensor except in the case when the axes of symmetry of the cubic are prescribed. However, the result established in theorem (4·1) partially resolves the problem of finding, for example, the cubic tensor nearest to a tetragonal polar elastic tensor in the following sense. If a tetragonal polar elastic tensor is referred to its natural coordinate system, only the first relation in (4·8) can fail to be satisfied. The last two relations are preserved under any rotation about the third axis and a suitable rotation about the third axis will yield a C_{16} and C_{26}

satisfying $(4\cdot8)_1$. The residue of **C** modulo its nearest cubic with symmetry axes which coincide with the new coordinate axes, will then be a local minimum.

5. Generalizations to other symmetry groups of crystals

It is well known that there are thirty-two different classes of crystals, which are among the most important anisotropic materials (Love, 1944). The symmetries of the various crystalline classes are described by the groups of covering operations which correspond to them. If we confine our attention only to the elastic tensors associated with the various classes, the thirty-two classes coalesce into nine groups. The elastic tensors of these nine groups are invariant under corresponding groups of orthogonal transformations. Table 1 contains an identification of these groups, the corresponding number of independent elastic constants and the name of a representative crystalline class, after Miers (Love, 1944).

Table 1. *Classification of crystals according to number of elastic constants*

Group	Name of representative class (after Miers)	Number of elastic constants
1	Asymmetric	21
2	Equatorial	13
3	Digonal holoaxial	9
4	Trigonal polar	7
5	Trigonal holoaxial	6
6	Hexagonal polar	5
7	Tetragonal polar	7
8	Tetragonal holoaxial	6
9	Tesseral polar (cubic)	3

By considering the invariant transformations of the nine groups, we see that they are subgroups of one another and of the isotropic group, as shown in Fig. 1, where the arrows show transitions from a group to a subgroup. The numbers in Fig. 1 correspond to the group number of Table 1.

The discussion in the preceding sections is applicable for finding the elastic tensor of some desired symmetry nearest to a given elastic tensor. If the symmetry group of the desired tensor is a subgroup of the symmetry group of the given tensor, then the nearest elastic tensor to the given tensor is the tensor itself. For example, the nearest asymmetric (triclinic) tensor to any elastic tensor is the tensor itself. However, a residue is obtained if, in Fig. 1, the group of the desired symmetry cannot be reached from the group of the given tensor by a sequence of arrows. As an example we give below the construction of a hexagonal polar tensor nearest to a tesseral polar (cubic) tensor. It may be mentioned that this construction may have certain practical applications in vibration problems in which factorization of the

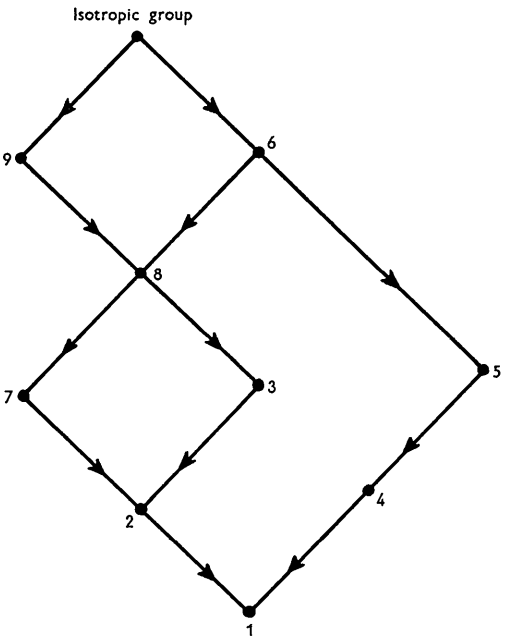

Fig. 1. Relation of the nine groups of Table 1 to each other and to the isotropic group.

frequency equation is possible in the case of hexagonal symmetry, but not in the case of cubic symmetry (Hearmon, 1961).

An orthonormal set of tensors for the hexagonal polar group is a set $\mathbf{A}_J$, $J=1$ to 5, where A_1 and A_2 are the isotropic tensors given in (3·5) and

$$\mathbf{A}_3 = \tfrac{1}{6}\begin{bmatrix} -2 & -2 & 1 & 0 & 0 & 0 \\ -2 & -2 & 1 & 0 & 0 & 0 \\ 1 & 1 & 4 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix},$$

$$\mathbf{A}_4 = \frac{1}{6\sqrt{30}}\begin{bmatrix} -8 & 4 & 4 & 0 & 0 & 0 \\ 4 & -8 & 4 & 0 & 0 & 0 \\ 4 & 4 & -8 & 0 & 0 & 0 \\ 0 & 0 & 0 & 9 & 0 & 0 \\ 0 & 0 & 0 & 0 & 9 & 0 \\ 0 & 0 & 0 & 0 & 0 & -6 \end{bmatrix},$$

$$\mathbf{A}_5 = \frac{1}{6\sqrt{6}}\begin{bmatrix} 1 & -5 & 4 & 0 & 0 & 0 \\ -5 & 1 & 4 & 0 & 0 & 0 \\ 4 & 4 & -8 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 3 \end{bmatrix}. \tag{5·1}$$

The nearest hexagonal polar tensor to a given cubic elastic tensor, constructed following the method of Section 2, is given by

$$c'_{ij} = \begin{bmatrix} \frac{1}{4}(3c_{11}+c_{12}+2c_{44}) & \frac{1}{4}(c_{11}+3c_{12}-2c_{44}) & c_{12} & 0 & 0 & 0 \\ \frac{1}{4}(c_{11}+3c_{12}-2c_{44}) & \frac{1}{4}(3c_{11}+c_{12}+2c_{44}) & c_{12} & 0 & 0 & 0 \\ c_{12} & c_{12} & c_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2}(c_{11}-c_{12}) \end{bmatrix}, \quad (5\cdot2)$$

where c_{11}, c_{12}, and c_{44} are the elastic constants of the cubic tensor.

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Stereochemistry of Arsenic. IX. Diiodomethylarsine*

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Crystals of diiodomethylarsine, CH_3AsI_2, are monoclinic with eight molecules in a unit cell of dimensions $a=14\cdot45$, $b=4\cdot60$, $c=19\cdot97$ Å, $\beta=114°20'$, space group $C2/c$. The structure has been determined from partial three-dimensional data in normal and generalized projections along b, and values of the bond distances, valency angles, and intermolecular separations have been obtained.

As part of a series of investigations of compounds containing arsenic, the crystal and molecular structure of diiodomethylarsine has been determined; it is one of the few simple arsenic derivatives which are solid at room temperature.

Experimental

Crystals of diiodomethylarsine, which are yellow-orange, are volatile and melt at about room temperature. For recording the X-ray data, crystals were sealed in capillaries and cooled by a stream of nitrogen which was first passed through a coil immersed in an ice-bath. The unit-cell dimensions and space group were determined from various rotation, oscillation, Weissenberg (Cu $K\alpha$) and precession (Mo $K\alpha$) films.

Crystal data (at 5–10 °C; λ(Cu $K\alpha$) = 1·5418 Å, λ(Mo $K\alpha$) = 0·7107 Å).

Diiodomethylarsine, CH_3AsI_2; M, 343·85; m.p. 26 °C.

Monoclinic,

$a=14\cdot45$, $b=4\cdot60$, $c=19\cdot97$ Å, $\beta=114°\,20'$.

$U=1209\cdot5$ Å^3.

D_x (with $Z=8$) = 3·8 g.cm^{-3}.

Absorption coefficient, μ(Cu $K\alpha$) = 939 cm^{-1}.

$F(000)=1184$.

Absent reflexions: hkl when $(h+k)$ is odd, $h0l$ when l is odd.

Space group is Cc or $C2/c$. Analysis has proceeded satisfactorily in $C2/c$.

No suitable flotation medium was available for measuring the density; the density of the liquid, measured at room temperature by means of a density bottle, was 3·1 g.cm^{-3}, and, since it seemed likely that the solid at slightly reduced temperatures would have a higher density, $Z=8$ was assumed. This was confirmed by the structure analysis.

Intensity data for the $h0l$ and $h1l$ reflexions were recorded on Weissenberg films and estimated visually, and the structure amplitudes were derived as usual, the absolute scale being established later by correlation with the calculated structure factors. The crystal used was a needle, elongated along b, with a rectangular cross-section 0·4 × 0·13 mm, the (001) face being developed. The films were textbook examples (Buerger, 1960) of severe absorption effects, and corrections were applied (Howells, 1950). These absorption correction factors applied to the intensities varied from 1 to about 150, and since they are approximate, the accuracy of the measured structure amplitudes is probably rather limited. 140 independent $h0l$ reflexions (77% of the possible) and 213 $h1l$ reflexions (62%) were observed.

* Part VIII: Camerman & Trotter (1963).