

In the use of this method as a setting method the main difficulty arises in selecting the reflexions to be brought into coincidence. This does not arise with irregular fragments of known unit cell (*e.g.* ground spheres), and the method may then prove superior to others. For example a colleague setting an irregular crystal of (?) face-centred cubic ferritungstite to [100] repeatedly converged on [111] by trial oscillation photographs. We had no difficulty in bringing two pairs of 111 reflexions into off-equatorial coincidence by this method, thus setting to the required axis. In some similar cases it may well happen that the predicted position of *A* in Fig. 1 lies outside the range of the arcs. The prediction will then be rather inaccurate owing to departures from the approximations above, but should suffice to indicate how the crystal should be remounted for a further triplet of trial rotation photographs. The indication of azimuth is likely to be more accurate than that of the inclination. It may be preferable to locate another known axis, accessible to the arcs, and derive the inclination from this.

Most workers use trial oscillation (or Laue) photographs for normal crystal setting, when using an irregular fragment. It is well known that recognizing badly missed layer lines is a knack, to be acquired by practice. The writer derived this method for general use before acquiring this knack, to study serendibite (Prior & Coomáraswámy, 1903; *cf.* Pertzév & Nikitina, 1959) available as type material in the form of rough irregular fragments thought to be triclinic. The

above method was triumphantly successful at first attempt, setting a crystal on to an axis displaying equatorial symmetry on even-order, but not on odd-order layer lines, by using off-equatorial coincidences. The axis proved to be [122] of the reduced all-acute triclinic cell.

Subsequent use suggests that this success was partly accidental. The difficulty lies in properly selecting the reflexions to be brought into coincidence. Choice of off-equatorial coincidences if possible will favour setting to a symmetry axis if any exists. It seems likely that extending Fig. 1 to consider more than two reflexions, thus obtaining a consensus, offers best chance of success. The method used in these circumstances is simple and offers as much chance of quick success as trial oscillation photographs, but for general setting of irregular fragments, the method of Brooker & Nuffield, while more elaborate, is more certain. However, where the unit cell of the irregular fragment is known, the present method offers many advantages over other recommended photographic methods.

#### References

- BROOKER, E. J. & NUFFIELD, E. W. (1966). *Acta Cryst.* **20**, 496.  
 PERTZEV, N. N. & NIKITINA, I. B. (1959). *Mem. All-Union Min. Soc.* **88**, 169. *cf. Miner. Abstracts* (1959), **14**, 274.  
 PRIOR, G. T. & COOMÁRASWÁMY, A. K. (1903). *Miner. Mag.* **13**, 224.  
 ROOF, R. B., JR (1955). *Acta Cryst.* **8**, 434.

*Acta Cryst.* (1968). **A24**, 273

## The Decomposition of an Anisotropic Elastic Tensor

BY YIH-O TU

*Thomas J. Watson Research Center, Yorktown Heights, New York, U.S.A.*

(Received 30 March 1967)

The classical theory of invariants asserts that there exists a finite integrity basis whose elements are polynomials of strain components and are invariant under the group of transformation defining each symmetry class of a crystal. By constructing a strain energy function made up of the elements of an integrity basis for a certain symmetry class, we derive a tensor basis which spans the space of elastic constants for crystals of this symmetry class. Introducing systematically new elements of the integrity basis into the construction of the strain energy function, we construct five hierarchies of orthonormal tensor bases which span the space of the second-order elastic constants of all crystal systems. Any elastic tensor of rank four possessing certain crystallographic symmetry may be decomposed into a sum of tensors of increasing symmetry. From this representation of an anisotropic elastic tensor, the tensor of any given symmetry, not only the isotropic one, nearest the given tensor can be read off immediately. Bases which span the space of elastic constants of orders higher than the second may be computed in a similar manner. Such computations can be carried out by a computer. A FORMAC program of 7090/94 IBSYS has been written to obtain the elastic constants of the second and the third order for each class of a crystal.

### 1. Introduction

In an investigation of the physical properties of an anisotropic body, one sometimes begins with the cor-

responding properties of an isotropic body having the same geometry and proximal constitutive physical relations, and for which some knowledge may be obtainable with relative ease. It may then be possible to

determine properties of the anisotropic body by the method of perturbation. Ways of defining and constructing the isotropic elastic tensor 'nearest' a given elastic tensor have been presented by Gazis, Tadjbakhsh & Toupin (1963). In this paper we construct orthonormal bases of tensors of rank four which span the space of elastic tensors possessing certain point-group symmetry of a crystal. The orientation of the Cartesian coordinates  $(x_1, x_2, x_3)$  conforms to the conventions in *IRE Standards on Piezoelectric Crystals* (Institute of Radio Engineers, 1949); namely,

Monoclinic	$x_2  y,$
Tetragonal, trigonal and hexagonal	$x_3  z, x_1  x,$
Orthorhombic and cubic	$x_1  x, x_2  y, x_3  z,$

where  $(x, y, z)$  are the natural axes of symmetry of the crystal.

General procedures for the construction of linearly independent tensors of rank  $2N$ ,  $N=2, 3, \dots$  possessing given symmetry, are presented in § 2. By means of these tensors, orthonormal bases of tensors of given symmetry can be constructed and are given in § 3. The elements of the orthonormal bases of tensors of rank four are exhibited in both tensor and abbreviated matrix indices. The correspondence between the tensor indices and matrix indices is as follows:

Tensor indices:	11 22 33 23,32 31,13 12,21
Matrix indices:	1 2 3 4 5 6 .

For the elastic stiffness tensor, we set

$$c_{ijkl} = c_{MNP} \quad (i, j, k, l = 1, 2, 3 \text{ and } M, N = 1, 2, \dots, 6).$$

However, for the elastic compliance tensor  $s_{ijkl}$ , factors of 2 and 4 are introduced as follows:

$$\begin{aligned} s_{ijkl} &= s_{MNP} \text{ when both } M \text{ and } N \text{ are } 1, 2 \text{ or } 3, \\ 2s_{ijkl} &= s_{MNP} \text{ when either } M \text{ or } N \text{ is } 4, 5 \text{ or } 6, \\ 4s_{ijkl} &= s_{MNP} \text{ when both } M \text{ and } N \text{ are } 4, 5 \text{ or } 6. \end{aligned}$$

Consequently, the matrix elements in § 3 must be multiplied by the factors 2 and 4 according to the above schemes.

To illustrate the method of decomposition, in § 4, the elastic stiffness tensor of quartz is decomposed into a sum of tensors of increasing symmetry. From this representation of an anisotropic elastic tensor, the tensor of any given symmetry, not only the isotropic one, nearest the given tensor can be read off immediately.

## 2. Invariant tensors

When a perfectly elastic crystal, initially stress-free, is deformed either isothermally or adiabatically to a final stressed state, the strain energy  $\bar{W}$  is a function of state. Furthermore,  $\bar{W}$  is invariant under the finite group of transformations,  $G$ , which defines the symmetry class of the crystal. For the purposes of this paper, it is assumed that  $\bar{W}$  is expressible as a polynomial in the

strain components  $E_{ij}$ . Accordingly, if  $||a_{ij}||$  is an element of  $G$ , and  $\bar{E}_{ij} = a_{ik}a_{jl}E_{kl}$ ,\* then it is required that

$$\bar{W}(\bar{E}_{ij}) = \bar{W}(E_{ij}), \quad (1)$$

for every  $||a_{ij}||$  in  $G$  and all values of  $E_{ij}$ . A classical result of the theory of invariants (Weyl, 1946) is the existence of a finite integrity basis  $\{I_1, I_2, \dots, I_k\}$  such that every polynomial function satisfying (1) is expressible as a polynomial in the elements of the integrity basis. Each element  $I_n$  of an integrity basis is itself a polynomial in  $E_{ij}$  satisfying (1). For the case of an isotropic material, for example, an integrity basis has three elements. They are polynomials of the first, second and third degree in  $E_{ij}$ , respectively, and may be chosen as follows:

$$\left. \begin{aligned} \text{I} &= \text{tr}(E_{ij}) = E_{ii} = E_{11} + E_{22} + E_{33} \\ \text{II} &= \frac{1}{2}[E_{ii}E_{jj} - E_{ij}E_{ij}] \\ &= (E_{11}E_{22} + E_{22}E_{33} + E_{33}E_{11}) - (E_{12}^2 + E_{23}^2 + E_{31}^2) \\ \text{III} &= \det(E_{ij}) = \frac{1}{6}[E_{ii}E_{jj}E_{kk} - 3E_{ii}E_{jk}E_{ki} \\ &\quad + 2E_{ij}E_{jk}E_{ki}] \\ &= E_{11}E_{22}E_{33} + 2E_{12}E_{23}E_{31} - (E_{11}E_{23}^2 + E_{22}E_{31}^2 \\ &\quad + E_{33}E_{12}^2) \end{aligned} \right\} (2)$$

Smith & Rivlin (1958) have determined the integrity basis for invariant functions of  $E_{ij}$  for each of the crystallographic point groups. Their results are summarized in Tables 1 and 2 for the purposes of the presentation of this paper. Table 1 gives the number of elements of an integrity-basis for each crystal class together with the number of the second- and third-order elastic constants. Table 2 gives some additional elements of polynomials of the first, second and third degree which are linearly independent of I, II and III of equations (2) as well as among themselves, together with the symmetry classes for which it is an invariant.

The second-order, third-order,  $\dots$ , elastic constants are tensors of ranks four, six,  $\dots$ , etc., and are defined and denoted by

$$\left. \begin{aligned} c_{ijkl} &= \left\{ \frac{\partial^2 \bar{W}}{\partial E_{ij} \partial E_{kl}} \right\} ||E_{ij}|| = ||0||, \\ c_{ijklmn} &= \left\{ \frac{\partial^3 \bar{W}}{\partial E_{ij} \partial E_{kl} \partial E_{mn}} \right\} ||E_{ij}|| = ||0||, \\ &\dots, \text{etc.} \end{aligned} \right\} (3)$$

These quantities are symmetric in the following pairs of indices,  $(i, j)$ ,  $(k, l)$ ,  $(m, n)$  and  $(ij, kl)$ ,  $(ij, mn)$ ,  $(kl, mn)$ . In particular,  $c_{ijkl}$  is called the elastic stiffness tensor. By choosing elements from Table 2 in addition to elements of (2), we shall form strain energy functions  $\bar{W}$  as polynomials of second and third degree in  $E_{ij}$ . Since polynomials of degree greater than three in the integrity basis do not contribute to the elastic tensors of ranks

\* The summation convention on the double indices of tensors is understood throughout this paper.

Table 1. Number of elastic constants and number of elements in an integrity basis for each crystal class

Crystal systems	Class symbols Schönflies International		Number of elements in an integrity basis						Number of elastic constants		
			1st degree	2nd degree	3rd degree	4th degree	5th degree	6th degree	2nd order	3rd order	
Triclinic	{	$C_1$	1	6	0	0	0	0	0	21	56
		$C_i$	$\bar{1}$	6	0	0	0	0	0	21	56
Monoclinic	{	$C_2$	2	4	3	0	0	0	0	13	32
		$C_s$	$m$	4	3	0	0	0	0	13	32
		$C_{2h}$	$2/m$	4	3	0	0	0	0	13	32
Orthorhombic	{	$D_2$	222	3	3	1	0	0	0	9	20
		$C_{2v}$	$mm2$	3	3	1	0	0	0	9	20
		$D_{2h}$	$mmm$	3	3	1	0	0	0	9	20
Tetragonal	{	$C_4$	4	2	4	4	2	0	0	7	16
		$S_4$	$\bar{4}$	2	4	4	2	0	0	7	16
		$C_{4h}$	$4/m$	2	4	4	2	0	0	7	16
		$D_4$	422	2	3	2	1	0	0	6	12
		$C_{4h}$	$4mm$	2	3	2	1	0	0	6	12
		$D_{2d}$	$\bar{4}2m$	2	3	2	1	0	0	6	12
Trigonal	{	$D_{4h}$	$4/mmm$	2	3	2	1	0	0	6	12
		$C_3$	3	2	4	8	0	0	0	7	20
		$C_{3i}$	$\bar{3}$	2	4	8	0	0	0	7	20
		$D_3$	32	2	3	4	0	0	0	6	14
		$C_{3v}$	$3m$	2	3	4	0	0	0	6	14
		$D_{3d}$	$\bar{3}m$	2	3	4	0	0	0	6	14
Hexagonal	{	$C_6$	6	2	2	4	2	2	2	5	12
		$C_{3h}$	$\bar{6}$	2	2	4	2	2	2	5	12
		$C_{6h}$	$6/m$	2	2	4	2	2	2	5	12
		$D_6$	622	2	2	2	1	1	1	5	10
		$C_{6v}$	$6mm$	2	2	2	1	1	1	5	10
		$D_{3h}$	$\bar{6}m2$	2	2	2	1	1	1	5	10
Cubic	{	$D_{6h}$	$6/mmm$	2	2	2	1	1	1	5	10
		$T$	23	1	2	5	3	2	1	3	8
		$T_h$	$m\bar{3}$	1	2	5	3	2	1	3	8
		$O$	432	1	2	3	2	1	0	3	6
		$T_d$	$\bar{4}3m$	1	2	3	2	1	0	3	6
		$O_h$	$m\bar{3}m$	1	2	3	2	1	0	3	6
Isotropic			1	1	1	0	0	0	2	3	

Table 2. First, second and third degree anisotropic polynomials and their invariant properties

	Polynomials	Invariance	
1st degree	{ $E_{33}$ $E_{11}$ $E_{31}$	Tetragonal, trigonal, hexagonal, orthorhombic, monoclinic Orthorhombic, monoclinic Monoclinic	
2nd degree	{ $E_{12}^2 + E_{23}^2 + E_{31}^2$ $E_{23}^2 + E_{31}^2$ $E_{12}(E_{11} - E_{22})$ $E_{23}(E_{11} - E_{22}) + 2E_{12}E_{31}$ $E_{31}(E_{11} - E_{22}) - 2E_{12}E_{23}$ $E_{23}^2$ $E_{12}E_{23}$	Tetragonal, cubic Tetragonal, trigonal, hexagonal, orthorhombic, monoclinic Tetragonal (classes 4, $\bar{4}$ , $4/m$ ) Trigonal Trigonal (classes 3, $\bar{3}$ ) Orthorhombic Monoclinic	
	3rd degree	{ $E_{11}E_{33}^2 + E_{22}E_{11}^2 + E_{33}E_{22}^2$ $E_{11}E_{31}^2 + E_{22}E_{12}^2 + E_{33}E_{23}^2$ $E_{11}E_{22}E_{33}$ $E_{12}E_{23}E_{31}$ $E_{23}E_{31}(E_{11} - E_{22})$ $E_{12}(E_{23}^2 - E_{31}^2)$ $E_{23}(E_{23}^2 - 3E_{31}^2)$ $E_{23}\{E_{11} + E_{22}\} + 4(E_{12}^2 - E_{22}^2) + 8E_{11}E_{12}E_{31}$ $E_{31}(E_{31}^2 - 3E_{23}^2)$ $E_{31}\{E_{11} + E_{22}\} + 4(E_{12}^2 - E_{22}^2) - 8E_{11}E_{12}E_{23}$ $E_{23}E_{31}(E_{11} - E_{22}) + E_{12}(E_{23}^2 - E_{31}^2)$ $3E_{12}(E_{11} - E_{22})^2 - 4E_{12}^3$ $E_{12}(E_{31}^2 - E_{23}^2) + E_{23}E_{31}(E_{22} - E_{33})$ $E_{11}\{E_{11} + 3E_{22}\} - 12E_{12}^2$	Cubic (classes 23, $m\bar{3}$ ) Cubic (classes 23, $m\bar{3}$ ) Cubic Cubic, tetragonal Tetragonal (classes 4, $\bar{4}$ , $4/m$ ) Tetragonal (classes 4, $\bar{4}$ , $4/m$ ) Trigonal Trigonal Trigonal (classes 3, $\bar{3}$ ) Trigonal (classes 3, $\bar{3}$ ) Trigonal (classes 3, $\bar{3}$ ) Trigonal (classes 3, $\bar{3}$ ) Trigonal (classes 3, $\bar{3}$ ), hexagonal (classes 6, $\bar{6}$ , $6/m$ ) Hexagonal (classes 6, $\bar{6}$ , $6/m$ ) Hexagonal, trigonal

four and six, as is evidenced from (3), such truncated polynomials of  $\bar{W}$  are sufficient for the determination of the second- and third-order elastic constants according to (3). In the following, we shall show the construction of bases in the space of the second-order elastic constants.

To begin with the isotropic integrity basis (2), the second-order elastic constants are obtained from terms of  $\mathbb{I}^2$  and  $\mathbb{II}$  of (2) in the strain energy  $\bar{W}$ . By carrying out the differentiations of (3), one obtains the following two isotropic tensors of rank four,

$$\left. \begin{aligned} \alpha_{ijkl} &= \delta_{ij}\delta_{kl} \\ \beta_{ijkl} &= \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk} \end{aligned} \right\} \quad (4)$$

We now introduce the element  $(E_{12}^2 + E_{23}^2 + E_{31}^2)$  of Table 2 into the construction of  $\bar{W}$ . Differentiation of the term involving this new element in  $\bar{W}$  gives the following tensor of rank four which is invariant under the group of transformations characterizing either a cubic or a tetragonal crystal,

$$\begin{aligned} \pi_{ijkl} &= (\delta_{i1}\delta_{j2} + \delta_{i2}\delta_{j1})(\delta_{k1}\delta_{l2} + \delta_{k2}\delta_{l1}) \\ &+ (\delta_{i2}\delta_{j3} + \delta_{i3}\delta_{j2})(\delta_{k2}\delta_{l3} + \delta_{k3}\delta_{l2}) \\ &+ (\delta_{i1}\delta_{j3} + \delta_{i3}\delta_{j1})(\delta_{k1}\delta_{l3} + \delta_{k3}\delta_{l1}) \end{aligned} \quad (5)$$

Consequently, the three elements  $(\alpha, \beta, \pi)$  of (4) and (5) constitute a tensor basis for the space of the second-order elastic constants of a cubic crystal. With the additional introduction of the elements  $E_{33}$  and  $(E_{23}^2 + E_{31}^2)$  of Table 2, the three additional second degree terms  $E_{33}^2$ ,  $E_{33}(E_{11} + E_{22} + E_{33})$  and  $(E_{23}^2 + E_{31}^2)$  in  $\bar{W}$  produce three more tensors of rank four in addition to  $(\alpha, \beta, \pi)$ ; they are

$$\left. \begin{aligned} \gamma_{ijkl} &= \delta_{i3}\delta_{j3}\delta_{k3}\delta_{l3} \\ \delta_{ijkl} &= \delta_{ij}\delta_{k3}\delta_{l3} + \delta_{i3}\delta_{j3}\delta_{kl} \\ \epsilon_{ijkl} &= (\delta_{i2}\delta_{j3} + \delta_{i3}\delta_{j2})(\delta_{k2}\delta_{l3} + \delta_{k3}\delta_{l2}) \\ &+ (\delta_{i1}\delta_{j3} + \delta_{i3}\delta_{j1})(\delta_{k1}\delta_{l3} + \delta_{k3}\delta_{l1}) \end{aligned} \right\} \quad (6)$$

Therefore, the six elements  $(\alpha, \beta, \pi, \gamma, \delta, \epsilon)$  of (4), (5) and (6) form a basis for the space of the second-order elastic constants of crystals of classes 422, 4mm,  $\bar{4}2m$  and 4/mmm in the tetragonal system. At the same time, the five elements  $(\alpha, \beta, \gamma, \delta, \epsilon)$  form a basis for the space of the second-order elastic constants of a hexagonal crystal.

By continuing the computations as outlined above, we obtain sixteen linearly independent tensors of rank four whose expressions are given in Table 3, together with the symmetry classes for which each is an invariant. Table 4 exhibits the use of these tensors to form five hierarchies of bases which span the space of second-order elastic constants for each symmetry class, together with the multiplication tables. The inner product of two tensors  $A_{ijkl}$  and  $B_{ijkl}$  which enters the multiplication table is defined as  $(\mathbf{A}, \mathbf{B}) = A_{ijkl}B_{ijkl}$ .

Bases which span the space of elastic constants of orders higher than the second may be computed in a similar manner. The tedious but straightforward algebraic procedures can best be handled by a computer using available symbolic manipulation programming such as FORMAC of 7090/94 IBSYS. In fact, the third-order elastic constants listed by Hearmon (1953) have been reproduced by a FORMAC program but with the additional feature of exhibiting hierarchies of bases similar to Table 4. As the number of the third-order elastic constants is so many, as evidenced in Table 1, details of the computer results will not be given here.

### 3. Orthonormal bases

By a linear combination of elements in a basis in Table 4, one can, instead, construct an orthonormal basis whose elements are (1) mutually orthogonal; *i.e.*  $(\mathbf{A}, \mathbf{B}) = 0$ , if  $A_{ijkl} \neq B_{ijkl}$ , and are (2) normal; *i.e.*  $(\mathbf{A}, \mathbf{A}) = 1$ , for elements  $A$  and  $B$  in the orthonormal basis. Twenty orthonormal tensors have been constructed. They are displayed in both their tensor forms and their matrix forms in Table 5, together with the

Table 3. *Tensors of rank four and their invariant properties*

Expression	Invariance
$\alpha_{ijkl} = \delta_{ij}\delta_{kl}$	Isotropic
$\beta_{ijkl} = \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}$	
$\pi_{ijkl} = (\delta_{i1}\delta_{j2} + \delta_{i2}\delta_{j1})(\delta_{k1}\delta_{l2} + \delta_{k2}\delta_{l1}) + (\delta_{i2}\delta_{j3} + \delta_{i3}\delta_{j2})(\delta_{k2}\delta_{l3} + \delta_{k3}\delta_{l2}) + (\delta_{i1}\delta_{j3} + \delta_{i3}\delta_{j1})(\delta_{k1}\delta_{l3} + \delta_{k3}\delta_{l1})$	Cubic, tetragonal, Orthorhombic, monoclinic
$\gamma_{ijkl} = \delta_{i3}\delta_{j3}\delta_{k3}\delta_{l3}$	
$\delta_{ijkl} = \delta_{ij}\delta_{k3}\delta_{l3} + \delta_{i3}\delta_{j3}\delta_{kl}$	Tetragonal, hexagonal, Trigonal, orthorhombic, Monoclinic
$\epsilon_{ijkl} = (\delta_{i2}\delta_{j3} + \delta_{i3}\delta_{j2})(\delta_{k2}\delta_{l3} + \delta_{k3}\delta_{l2}) + (\delta_{i1}\delta_{j3} + \delta_{i3}\delta_{j1})(\delta_{k1}\delta_{l3} + \delta_{k3}\delta_{l1})$	
$\varphi_{ijkl} = (\delta_{i1}\delta_{j2} + \delta_{i2}\delta_{j1})(\delta_{k1}\delta_{l3} + \delta_{k3}\delta_{l1}) + (\delta_{i1}\delta_{j3} + \delta_{i3}\delta_{j1})(\delta_{k1}\delta_{l2} + \delta_{k2}\delta_{l1}) + (\delta_{i2}\delta_{j3} + \delta_{i3}\delta_{j2})(\delta_{k1}\delta_{l1} - \delta_{k2}\delta_{l2}) + (K_{i1}\delta_{j1} - \delta_{i2}\delta_{j2})(\delta_{k2}\delta_{l3} + \delta_{k3}\delta_{l2})$	Trigonal
$\psi_{ijkl} = (\delta_{i1}\delta_{j3} + \delta_{i3}\delta_{j1})(\delta_{k1}\delta_{l1} - \delta_{k2}\delta_{l2}) + (\delta_{i1}\delta_{j1} - \delta_{i2}\delta_{j2})(\delta_{k1}\delta_{l3} + \delta_{k3}\delta_{l1}) - (\delta_{i1}\delta_{j2} + \delta_{i2}\delta_{j1})(\delta_{k2}\delta_{l3} + \delta_{k3}\delta_{l2}) - (\delta_{i2}\delta_{j3} + \delta_{i3}\delta_{j2})(\delta_{k1}\delta_{l2} + \delta_{k2}\delta_{l1})$	
$\omega_{ijkl} = (\delta_{i1}\delta_{j2} + \delta_{i2}\delta_{j1})(\delta_{k1}\delta_{l1} - \delta_{k2}\delta_{l2}) + (\delta_{i1}\delta_{j1} - \delta_{i2}\delta_{j2})(\delta_{k1}\delta_{l2} + \delta_{k2}\delta_{l1})$	Tetragonal (classes 4, $\bar{4}$ , 4/m)
$\varrho_{ijkl} = \delta_{i1}\delta_{j1}\delta_{k1}\delta_{l1}$	
$\theta_{ijkl} = (\delta_{i2}\delta_{j3} + \delta_{i3}\delta_{j2})(\delta_{k2}\delta_{l3} + \delta_{k3}\delta_{l2})$	Orthorhombic, monoclinic
$\sigma_{ijkl} = (\delta_{i3}\delta_{j3}\delta_{k1}\delta_{l1} + \delta_{i1}\delta_{j1}\delta_{k3}\delta_{l3})$	
$\lambda_{ijkl} = (\delta_{i2}\delta_{j3} + \delta_{i3}\delta_{j2})(\delta_{k1}\delta_{l2} + \delta_{k2}\delta_{l1}) + (\delta_{i1}\delta_{j2} + \delta_{i2}\delta_{j1})(\delta_{k2}\delta_{l3} + \delta_{k3}\delta_{l2})$	Monoclinic
$\mu_{ijkl} = (\delta_{i1}\delta_{j3} + \delta_{i3}\delta_{j1})\delta_{k3}\delta_{l3} + \delta_{i3}\delta_{j3}(\delta_{k1}\delta_{l3} + \delta_{k3}\delta_{l1})$	
$\tau_{ijkl} = (\delta_{i1}\delta_{j3} + \delta_{i3}\delta_{j1})\delta_{k1}\delta_{l1} + \delta_{i1}\delta_{j1}(\delta_{k1}\delta_{l3} + \delta_{k3}\delta_{l1})$	
$\zeta_{ijkl} = (\delta_{i1}\delta_{j3} + \delta_{i3}\delta_{j1})\delta_{k2}\delta_{l2} + \delta_{i2}\delta_{j2}(\delta_{k1}\delta_{l3} + \delta_{k3}\delta_{l1})$	

symmetry classes for which each is an invariant. Table 6 exhibits the five hierarchies of orthonormal tensor bases which span the space of the second-order elastic constants.

Any elastic tensor of rank four possessing certain crystallographic symmetry may be decomposed ac-

ording to one of the schemes in Table 6. Thus the elastic stiffness tensor of crystals of classes  $3, \bar{3}$ , for example, can be represented in the form

$$c_{ijkl} = \sum_{K=1}^{VII} (c, A^K) A_{ijkl}^K, \quad (7)$$

Table 4. Five hierarchies of tensor bases and multiplication tables

		Trigonal ( $3, \bar{3}$ )						
		Trigonal ( $32, 3m, \bar{3}m$ )						
		Hexagonal						
		Isotropic						
		$\alpha$	$\beta$	$\gamma$	$\delta$	$\varepsilon$	$\varphi$	$\psi$
(a)	$\alpha$	9	6	1	6	0	0	0
	$\beta$		24	2	4	8	0	0
	$\gamma$			1	2	0	0	0
	$\delta$				8	0	0	0
	$\varepsilon$					8	0	0
	$\varphi$						16	0
	$\psi$							16
		Tetragonal ( $4, \bar{4}, 4/m$ )						
		Tetragonal ( $422, 4mm, \bar{4}2m, 4/mmm$ )						
		Cubic						
		Isotropic						
		$\alpha$	$\beta$	$\pi$	$\gamma$	$\delta$	$\varepsilon$	$\omega$
(b)	$\alpha$	9	6	0	1	6	0	0
	$\beta$		24	12	2	4	8	0
	$\pi$			12	0	0	8	0
	$\gamma$				1	2	0	0
	$\delta$					8	0	0
	$\varepsilon$						8	0
	$\omega$							8
		Tetragonal ( $4, \bar{4}, 4/m$ )						
		Tetragonal ( $422, 4mm, \bar{4}2m, 4/mmm$ )						
		Hexagonal						
		Isotropic						
		$\alpha$	$\beta$	$\gamma$	$\delta$	$\varepsilon$	$\pi$	$\omega$
(c)	$\alpha$	9	6	1	6	0	0	0
	$\beta$		24	2	4	8	12	0
	$\gamma$			1	2	0	0	0
	$\delta$				8	0	0	0
	$\varepsilon$					8	8	0
	$\pi$						12	0
	$\omega$							8
		Orthorhombic						
		Tetragonal ( $422, 4mm, \bar{4}2m, 4/mmm$ )						
		Hexagonal						
		Isotropic						
		$\alpha$	$\beta$	$\gamma$	$\delta$	$\varepsilon$	$\pi$	$\varrho$
		$\sigma$	$\theta$	$\lambda$	$\mu$	$\tau$	$\zeta$	
(d)	$\alpha$	9	6	1	6	0	0	1
	$\beta$		24	2	4	8	12	2
	$\gamma$			1	2	0	0	0
	$\delta$				8	0	0	2
	$\varepsilon$					8	0	0
	$\pi$						12	0
	$\varrho$							1
	$\sigma$							2
	$\theta$							4
	$\lambda$							8
	$\mu$							4
	$\tau$							4
	$\zeta$							4

Table 4 (cont.)

(e)	Orthorhombic										Monoclinic			
	Tetragonal (422, 4mm, 42m, 4/mmm)													
	Cubic													
	Isotropic													
	$\alpha$	$\beta$	$\pi$	$\gamma$	$\delta$	$\varepsilon$	$\varrho$	$\sigma$	$\theta$	$\lambda$	$\mu$	$\tau$	$\zeta$	
$\alpha$	9	6	0	1	6	0	1	2	0	0	0	0	0	
$\beta$		24	12	2	4	8	2	0	4	0	0	0	0	
$\pi$			12	0	0	8	0	0	4	0	0	0	0	
$\gamma$				1	2	0	0	0	0	0	0	0	0	
$\delta$					8	0	0	2	0	0	0	0	0	
$\varepsilon$						8	0	0	4	0	0	0	0	
$\varrho$							1	0	0	0	0	0	0	
$\sigma$								2	0	0	0	0	0	
$\theta$									4	0	0	0	0	
$\lambda$										8	0	0	0	
$\mu$											4	0	0	
$\tau$												4	0	
$\zeta$													4	

Table 5. Orthonormal tensors of rank four, their matrix representations and their invariant properties

Name	Symmetry classes	Tensor	Matrix
$A^I$	Isotropic	$A_{ijkl}^I = \frac{1}{3}\alpha_{ijkl}$	$A_{IJ}^I = \frac{1}{3} \begin{pmatrix} 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$
$A^{II}$	Isotropic	$A_{ijkl}^{II} = \frac{1}{6\sqrt{5}} [3\beta_{ijkl} - 2\alpha_{ijkl}]$	$A_{IJ}^{II} = \frac{1}{6\sqrt{5}} \begin{pmatrix} 4 & -2 & -2 & 0 & 0 & 0 \\ -2 & 4 & -2 & 0 & 0 & 0 \\ -2 & -2 & 4 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 3 \end{pmatrix}$
$A^C$	Cubic Tetragonal Orthorhombic Monoclinic	$A_{ijkl}^C = \frac{1}{2\sqrt{30}} [5\pi_{ijkl} - 3\beta_{ijkl} + 2\alpha_{ijkl}]$	$A_{IJ}^C = \frac{1}{\sqrt{30}} \begin{pmatrix} -2 & 1 & 1 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 & 0 \\ 1 & 1 & -2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$
$A^{H1}$	Tetragonal Hexagonal Trigonal Orthorhombic Monoclinic	$A_{ijkl}^{H1} = \frac{1}{6\sqrt{5}} [15\gamma_{ijkl} - \beta_{ijkl} - \alpha_{ijkl}]$	$A_{IJ}^{H1} = \frac{1}{6\sqrt{5}} \begin{pmatrix} -3 & -1 & -1 & 0 & 0 & 0 \\ -1 & -3 & -1 & 0 & 0 & 0 \\ -1 & -1 & -3 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 \end{pmatrix}$
$A^{H2}$	Tetragonal Hexagonal Trigonal Orthorhombic Monoclinic	$A_{ijkl}^{H2} = \frac{1}{12} [9\delta_{ijkl} - 15\gamma_{ijkl} + \beta_{ijkl} - 5\alpha_{ijkl}]$	$A_{IJ}^{H2} = \frac{1}{12} \begin{pmatrix} -3 & -5 & 4 & 0 & 0 & 0 \\ -5 & -3 & 4 & 0 & 0 & 0 \\ 4 & 4 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$
$A^{H3}$	Tetragonal Hexagonal Trigonal Orthorhombic Monoclinic	$A_{ijkl}^{H3} = \frac{1}{4} [2\varepsilon_{ijkl} - \delta_{ijkl} + 3\gamma_{ijkl} - \beta_{ijkl} + \alpha_{ijkl}]$	$A_{IJ}^{H3} = \frac{1}{4} \begin{pmatrix} -1 & 1 & 0 & 0 & 0 & 0 \\ 1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 \end{pmatrix}$
$A^{TH}$	Tetragonal Orthorhombic Monoclinic	$A_{ijkl}^{TH} = \frac{1}{2\sqrt{2}} [2\pi_{ijkl} - \varepsilon_{ijkl} - \delta_{ijkl} + 3\gamma_{ijkl} - \beta_{ijkl} + \alpha_{ijkl}]$	$A_{IJ}^{TH} = \frac{1}{2\sqrt{2}} \begin{pmatrix} -1 & 1 & 0 & 0 & 0 & 0 \\ 1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$

Table 5 (cont.)

Name	Symmetry classes	Tensor	Matrix
$A^{TC1}$	Tetragonal Orthorhombic Monoclinic	$A_{ijkl}^{TC1} = \frac{1}{\sqrt{6}} [3\gamma_{ijkl} + \frac{1}{2}\pi_{ijkl} - \frac{1}{2}\beta_{ijkl}]$	$A_{IJ}^{TC1} = \frac{1}{\sqrt{6}} \begin{pmatrix} -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$
$A^{TC2}$	Tetragonal Orthorhombic Monoclinic	$A_{ijkl}^{TC2} = \frac{1}{2\sqrt{3}} [3\delta_{ijkl} - 6\gamma_{ijkl} - \pi_{ijkl} + \beta_{ijkl} - 2\alpha_{ijkl}]$	$A_{IJ}^{TC2} = \frac{1}{2\sqrt{3}} \begin{pmatrix} 0 & -2 & 1 & 0 & 0 & 0 \\ -2 & 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$
$A^{TC3}$	Tetragonal Orthorhombic Monoclinic	$A_{ijkl}^{TC3} = \frac{1}{2\sqrt{6}} [3\epsilon_{ijkl} - 2\pi_{ijkl}]$	$A_{IJ}^{TC3} = \frac{1}{2\sqrt{6}} \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -2 \end{pmatrix}$
$A^{TET}$	Tetragonal (classes $4, \bar{4}, 4/m$ )	$A_{ijkl}^{TET} = \frac{1}{2\sqrt{2}} \omega_{ijkl}$	$A_{IJ}^{TET} = \frac{1}{2\sqrt{2}} \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & -1 & 0 & 0 & 0 & 0 \end{pmatrix}$
$A^{TR1}$	Trigonal	$A_{ijkl}^{TR1} = \frac{1}{4}\phi_{ijkl}$	$A_{IJ}^{TR1} = \frac{1}{4} \begin{pmatrix} 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}$
$A^{TR2}$	Trigonal (classes $3, \bar{3}$ )	$A_{ijkl}^{TR2} = \frac{1}{4}\psi_{ijkl}$	$A_{IJ}^{TR2} = \frac{1}{4} \begin{pmatrix} 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 \\ 1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \end{pmatrix}$
$A^{VII}$	Orthorhombic Monoclinic	$A_{ijkl}^{VII} = \frac{1}{\sqrt{2}} [2\varrho_{ijkl} + \frac{1}{2}\pi_{ijkl} + \gamma_{ijkl} - \frac{1}{2}\beta_{ijkl}]$	$A_{IJ}^{VII} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$
$A^{VIII}$	Orthorhombic Monoclinic	$A_{ijkl}^{VIII} = \frac{1}{2} [2\sigma_{ijkl} - \delta_{ijkl} + 2\gamma_{ijkl}]$	$A_{IJ}^{VIII} = \frac{1}{2} \begin{pmatrix} 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 \\ 1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$
$A^{IX}$	Orthorhombic Monoclinic	$A_{ijkl}^{IX} = \frac{1}{2\sqrt{2}} [2\theta_{ijkl} - \epsilon_{ijkl}]$	$A_{IJ}^{IX} = \frac{1}{2\sqrt{2}} \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$
$A^X$	Monoclinic	$A_{ijkl}^X = \frac{1}{2\sqrt{2}} \lambda_{ijkl}$	$A_{IJ}^X = \frac{1}{2\sqrt{2}} \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix}$

Table 5 (cont.)

Name	Symmetry classes	Tensor	Matrix
$A^{XI}$	Monoclinic	$A_{ijkl}^{XI} = \frac{1}{2}\mu_{ijkl}$	$A_{IJ}^{XI} = \frac{1}{2} \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$
$A^{XII}$	Monoclinic	$A_{ijkl}^{XII} = \frac{1}{2}\tau_{ijkl}$	$A_{IJ}^{XII} = \frac{1}{2} \begin{pmatrix} 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \end{pmatrix}$
$A^{XIII}$	Monoclinic	$A_{ijkl}^{XIII} = \frac{1}{2}\zeta_{ijkl}$	$A_{IJ}^{XIII} = \frac{1}{2} \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$

Table 6. Five hierarchies of orthonormal bases

	$A^I$	$A^{II}$	$A^{III}$	$A^{IV}$	$A^V$	$A^{VI}$	$A^{VII}$	$A^{VIII}$	$A^{IX}$	$A^X$	$A^{XI}$	$A^{XII}$	$A^{XIII}$	
(a)	$A^I$	$A^{II}$	$A^{H1}$	$A^{H2}$	$A^{H3}$	$A^{TR1}$	$A^{TR2}$							
	— Isotropic —		Hexagonal											
			Trigonal ( $32, 3m, \bar{3}m$ )											
			Trigonal ( $3, \bar{3}$ )											
(b)	$A^I$	$A^{II}$	$A^C$	$A^{TC1}$	$A^{TC2}$	$A^{TC3}$	$A^{TET}$							
	— Isotropic —		Cubic											
			Tetragonal ( $422, 4mm, \bar{4}2m, 4/mmm$ )											
			Tetragonal ( $4, \bar{4}, 4/m$ )											
(c)	$A^I$	$A^{II}$	$A^{H1}$	$A^{H2}$	$A^{H3}$	$A^{TH}$	$A^{TET}$							
	— Isotropic —		Hexagonal											
			Tetragonal ( $422, 4mm, \bar{4}2m, 4/mmm$ )											
			Tetragonal ( $4, \bar{4}, 4/m$ )											
(d)	$A^I$	$A^{II}$	$A^{H1}$	$A^{H2}$	$A^{H3}$	$A^{TH}$	$A^{VII}$	$A^{VIII}$	$A^{IX}$	$A^X$	$A^{XI}$	$A^{XII}$	$A^{XIII}$	
	— Isotropic —		Hexagonal											
			Tetragonal ( $422, 4mm, \bar{4}2m, 4/mmm$ )											
			Orthorhombic											
								Monoclinic						
(e)	$A^I$	$A^{II}$	$A^C$	$A^{TC1}$	$A^{TC2}$	$A^{TC3}$	$A^{VII}$	$A^{VIII}$	$A^{IX}$	$A^X$	$A^{XI}$	$A^{XII}$	$A^{XIII}$	
	— Isotropic —		Cubic											
			Tetragonal ( $422, 4mm, \bar{4}2m, 4/mmm$ )											
			Orthorhombic											
								Monoclinic						

where  $A^K, K=I, II, \dots, VII$  are the orthonormal basis according to Table 6 (a), and  $(c, A^K)$  is the inner product of  $c_{ijkl}$  and  $A_{ijkl}^K$ . Likewise, the elastic stiffness tensor of classes  $4, \bar{4}$  and  $4/m$  crystals may be represented in the same form as (7) but with  $A^K$  chosen to

be the orthonormal basis according to either (b) or (c) of Table 6.

In order to facilitate the computation of inner products of an arbitrary elastic stiffness tensor  $c_{ijkl}$  and an element of an orthonormal basis, Table 7 lists the



Table 7. Formulas for the computation of inner products in terms of matrix elements

$$S_1 = \sum_{I=1}^3 c_{II}, \quad S_2 = \sum_{I=4}^6 s_{II}, \quad S_3 = \sum_{I=1}^3 \sum_{J=1}^3 c_{IJ}$$

$$(c, A^I) = \frac{1}{3} S_3$$

$$(c, A^{II}) = \frac{1}{3\sqrt{5}} [3S_1 + 6S_2 - S_3]$$

$$(c, A^C) = \frac{1}{\sqrt{30}} [4S_2 - 3S_1 + S_3]$$

$$(c, A^{H1}) = \frac{1}{6\sqrt{5}} [15c_{33} - 2S_1 - 4S_2 - S_3]$$

$$(c, A^{H2}) = \frac{1}{\sqrt{2}} [18(c_{13} + c_{23}) + 3c_{33} + 2S_1 + 4S_2 - 5S_3]$$

$$(c, A^{H3}) = \frac{1}{4} [8(c_{44} + c_{55}) - 2(c_{13} + c_{23}) + c_{33} - 2S_1 - 4S_2 + S_3]$$

$$(c, A^{TH}) = \frac{1}{2\sqrt{2}} [4c_{66} - 2(c_{13} + 2c_{23}) + c_{33} - 2S_1 + S_3]$$

$$(c, A^{TC1}) = \frac{1}{\sqrt{6}} [3c_{33} - S_1]$$

Table 7 (cont.)

$$S_1 = \sum_{I=1}^3 c_{II}, \quad S_2 = \sum_{I=4}^6 s_{II}, \quad S_3 = \sum_{I=1}^3 \sum_{J=1}^3 c_{IJ}$$

$$(c, A^{TC2}) = \frac{1}{\sqrt{3}} [3(c_{13} + c_{23}) + S_1 - S_3]$$

$$(c, A^{TC3}) = \sqrt{2/3} [c_{44} + c_{55} - 2c_{66}]$$

$$(c, A^{TEI}) = \sqrt{2} (c_{16} - c_{26})$$

$$(c, A^{TR1}) = 2c_{56} + c_{14} - c_{24}$$

$$(c, A^{TR2}) = c_{15} - c_{25} - 2c_{46}$$

$$(c, A^{VII}) = \frac{1}{\sqrt{2}} [c_{11} - c_{22}]$$

$$(c, A^{VIII}) = c_{13} - c_{23}$$

$$(c, A^{IX}) = \sqrt{2} [c_{44} - c_{55}]$$

$$(c, A^X) = 2\sqrt{2} c_{46}$$

$$(c, A^{XI}) = 2c_{35}$$

$$(c, A^{XII}) = 2c_{15}$$

$$(c, A^{XIII}) = 2c_{25}$$

formulas in terms of matrix elements  $c_{IJ}, I, J = 1, 2, \dots, 6$ . However, for the elastic compliance tensor  $s_{ijkl}$ , the coefficients in the formulas must be divided by 2 when either  $I$  or  $J$  of  $s_{IJ}$  is 4, 5, 6 and by 4 when both  $I$  and  $J$  of  $s_{IJ}$  are 4, 5 or 6.

$$c_{IJ} = \begin{pmatrix} 8.680 & 0.704 & 1.191 & -1.804 & 0 & 0 \\ 0.704 & 8.680 & 1.191 & 1.804 & 0 & 0 \\ 1.191 & 1.191 & 10.575 & 0 & 0 & 0 \\ -1.804 & 1.804 & 0 & 5.820 & 0 & 0 \\ 0 & 0 & 0 & 0 & 5.820 & -1.804 \\ 0 & 0 & 0 & 0 & -1.804 & 3.988 \end{pmatrix} \quad (12)$$

We now define and denote the norm of  $c_{ijkl}$  by

$$\|c\| = \{c_{ijkl} \cdot c_{ijkl}\}^{\frac{1}{2}}. \quad (8)$$

When  $c_{ijkl}$  is in the space spanned by the orthonormal basis  $\{A^K\}$ , it is easy to see that

$$\|c\| = \left\{ \sum_K (c, A^K) \right\}^{\frac{1}{2}}. \quad (9)$$

The nearest isotropic tensor, denoted by  $c_{ijkl}^0$  of  $c_{ijkl}$  is therefore

$$c_{ijkl}^0 = \sum_{K=1}^{\Pi} (c, A^K) A_{ijkl}^K \quad (10)$$

$$c_{IJ} = \begin{pmatrix} 10.250 & 2.726 & -0.803 & 0 & -0.929 & 0 \\ 2.726 & 8.680 & -0.831 & 0 & 0.388 & 0 \\ -0.803 & -0.831 & 12.992 & 0 & -0.577 & 0 \\ 0 & 0 & 0 & 2.895 & 0 & -0.243 \\ -0.929 & 0.388 & -0.577 & 0 & 3.825 & 0 \\ 0 & 0 & 0 & -0.243 & 0 & 6.912 \end{pmatrix} \quad (14)$$

which has a norm

$$\|c^0\| = \left\{ \sum_{K=1}^{\Pi} (c^0, A^K) \right\}^{\frac{1}{2}}. \quad (11)$$

In a similar manner, with respect to the tensor  $c_{ijkl}$ , the nearest tensors of other symmetry classes within the class spanned by the basis  $\{A^K\}$  may be read off readily from the representation, and their norms may be computed according to (9).

#### 4. Example

According to McSkimin, Andreatch & Thurston (1965), the elastic stiffness matrix  $c_{IJ}$  at room temperature of quartz (class 32) is given by

in  $10^{11}$  dyn.cm<sup>-2</sup>. Using scheme (a) of Table 6, the above matrix may be represented in the form

$$c_{IJ} = 11.368A^I + 21.386A^{II} + 0.457A^{H1} + 1.870A^{H2} + 3.663A^{H3} - 7.216A^{TR1}. \quad (13)$$

For an AT-cut quartz plate ( $yxl$ )  $35^\circ$ , if we orient the Cartesian coordinates in such a way that the  $(x_1, x_2)$ -plane lies on the middle plane of the plate and  $x_2 \parallel x$ , the matrix (12), referred to the new coordinates, becomes

which possesses the symmetry of the monoclinic system. This matrix may be represented in either of the following two ways according to scheme (d) or (e) of Table 6.

$$c_{IJ} = 11.368A^I + 21.386A^{II} + \left\{ \begin{array}{l} 3.160A^{H1} - 3.549A^{H2} - 3.560A^{H3} + 5.010A^{TH} \\ -1.301A^C + 2.880A^{TC1} - 4.091A^{TC2} - 5.800A^{TC3} \end{array} \right\} + 1.110A^{VII} + 0.027A^{VIII} - 1.315A^{IX} - 0.689A^X - 1.155A^{XI} - 1.859A^{XII} + 0.776A^{XIII}. \quad (15)$$

The nearest tensors of higher symmetry may be read off from equations (13) or (15). In particular, the nearest isotropic tensor,  $c_{ijkl}^0$ , being an invariant, has the following matrix:

$$c_{IJ}^0 = \begin{pmatrix} 10.165 & 0.601 & 0.601 & 0 & 0 & 0 \\ 0.601 & 10.165 & 0.601 & 0 & 0 & 0 \\ 0.601 & 0.601 & 10.165 & 0 & 0 & 0 \\ 0 & 0 & 0 & 4.782 & 0 & 0 \\ 0 & 0 & 0 & 0 & 4.782 & 0 \\ 0 & 0 & 0 & 0 & 0 & 4.782 \end{pmatrix}. \quad (16)$$

Define the number  $\varepsilon^0$  by

$$\varepsilon^0 = \frac{\|c\| - \|c^0\|}{\|c\|}. \quad (17)$$

$\varepsilon^0$  is a scalar constant independent of the rotation of the axes. It is a measure of 'nearness' of the nearest isotropic tensor. The value of  $\varepsilon^0$  for quartz at room-temperature is found to be 0.054. The use of  $\varepsilon^0$  as a perturbation parameter is currently being investigated

in a perturbation scheme of plane stress problems in anisotropic theory of elasticity.

The author is indebted to Dr R.A. Toupin for his criticism and help.

#### References

- GAZIS, D. C., TADJBAKHSI, I. & TOUPIN, R. A. (1963). *Acta Cryst.* **16**, 917.  
 HEARMON, R. F. S. (1953). *Acta Cryst.* **6**, 331.  
 INSTITUTE OF RADIO ENGINEERS (1949). *Proc. Inst. Radio Engrs. N.Y.*, **37**.  
 MCSKIMIN, H. J., ANDREATCH, P. & THURSTON, R. N. (1965). *J. of Appl. Phys.* **36**, 1624.  
 SMITH, G. F. & RIVLIN, R. S. (1958). *Trans. Amer. Math. Soc.* **88**, 175.  
 WEYL, H. (1946). *The Classical Groups, Their Invariants and Representations*. Princeton Univ. Press.

*Acta Cryst.* (1968). A24, 282

### The Atomic Mechanism of the Body-Centred Cubic to $\sigma$ -Phase Transformation

By W. J. KITCHINGMAN

*Metallurgy Department, University of Manchester Institute of Science and Technology, Sackville Street, Manchester 1, England*

(Received 12 June 1967)

An atomic mechanism for the body-centred cubic to  $\sigma$ -phase transformation is suggested. Atomic movements over small distances in the  $[11\bar{1}]_{b.c.c.}$  direction take place leading to the formation of a new layer structure. The transformation is completed by rotation of alternate layers of hexagons within zones related to kagomé tile structures. The mechanism suggests that certain groups of atoms are more strongly bonded in the  $[11\bar{1}]$  direction than others. The mechanism also suggests that the body-centred cubic phase exhibits partial long range order prior to the transformation. The ductility of  $\beta$ -uranium and the brittleness of FeCr and 2NbAl alloys is discussed in terms of the ordering and coordination numbers of the atomic positions in the  $\sigma$  structure.

#### Introduction

The occurrence of the  $\sigma$  phase and its properties have been reviewed by Hall & Algie (1966). The  $\sigma$  phase

always contains at least one transition group element. In alloys it is one of a series of phases occurring with the passage from the more open body-centred cubic structure to the closer packed hexagonal and face-

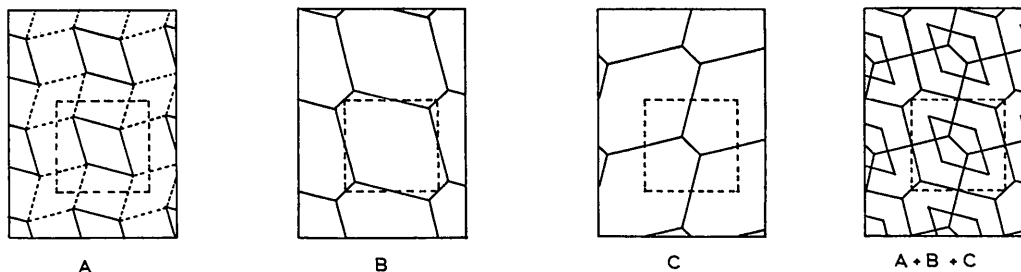


Fig. 1. The  $\sigma$ -phase structure described as a layer structure of kagomé tiles and diamond nets. The outline of the unit cell is also shown.