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A Simplified Calculation for the Elastic Constants of Arbitrarily Oriented Single Crystals

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(*Received* 22 *June* 1954 *and in revised form* 25 *December* 1955)

A simple, competely general, and easily remembered scheme is presented for solving problems involving the transformation of elastic constants from one orthogonal coordinate system to another rotated with respect to the first. Since the components of stress can be expressed as the elements of a second rank tensor, and the components of strain (if properly defined) can likewise be expressed as the elements of a second rank tensor, the elastic constants connecting stress and strain must be the elements of a fourth rank tensor. The method depends upon the simultaneous contraction of the fourth rank tensor and the quadratic products of the direction cosines connecting the two axis systems. The application of the resultant 'transformation matrix', instead of the conventional methods, reduces the number of steps to a minimum with a corresponding reduction in the chance for errors in the computation. The saving in time and labor is considerable, as is shown by typical examples.

1. Introduction

In many solid-state experiments on single crystals (e.g., the determination of elastic constants) it is necessary to express the elastic moduli or elastic constants in an axis system rotated with respect to an orthogonal system oriented along the principal crystallographic directions of the crystal. The matrix of the direction cosines connecting an arbitrary axis system (primed) in the specimen with this crystal-axis system (unprimed) can usually be determined in a straightforward manner (e.g., by X-ray analysis). Then if a system of stresses is applied to the specimen and the resultant strains are measured, the elastic constants of the material (relative to the unprimed system) can be calculated.

Difficulties in practice often arise due to the necessity for contracting a fourth rank tensor, and the

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cumbersome summation process involved. Further difficulties are encountered because the matrix of the strains does not transform as a second rank tensor with the strain elements defined in the usual manner. There are factors of $\frac{1}{2}$, 2 etc. that must be inserted at various points in the summation or in the tensor terms if the results are to agree with the elastic constants usually stated in the generalized form of Hooke's Law.

A simple, completely general, and easily remembered scheme for solving such problems is here presented. The following outline constitutes a set of directions for calculating elastic constants in a rotated axis system; the mathematical development of the method will be found in § 3.

2. The simplified calculation

(*A*) *The elastic constants*

1. Determine (experimentally) the direction cosines connecting the two unitary orthogonal axis systems and write them in the following array:

	x_1	x_2	x_3
x_1'	β_{11}	β_{12}	β_{13}
x_2'	β_{21}	β_{22}	β_{23}
x_3'	β_{31}	β_{32}	β_{33}

(1)

i.e. the matrix form of the three linear equations

$$x_1' = \beta_{11}x_1+\beta_{12}x_2+\beta_{13}x_3, \text{ etc.}$$

2. Write the quadratic combinations of the direction cosines in the following 6×6 array (which is defined as the matrix γ):

$$\gamma = \begin{bmatrix} \beta_{11}^2 & \beta_{12}^2 & \beta_{13}^2 & \beta_{12}\beta_{13} & \beta_{13}\beta_{11} & \beta_{11}\beta_{12} \\ \beta_{21}^2 & \beta_{22}^2 & \beta_{23}^2 & \beta_{22}\beta_{23} & \beta_{23}\beta_{21} & \beta_{21}\beta_{22} \\ \beta_{31}^2 & \beta_{32}^2 & \beta_{33}^2 & \beta_{32}\beta_{33} & \beta_{33}\beta_{31} & \beta_{31}\beta_{32} \\ 2\beta_{21}\beta_{31} & 2\beta_{22}\beta_{32} & 2\beta_{23}\beta_{33} & \begin{pmatrix}\beta_{22}\beta_{33}^{+}\\ \beta_{23}\beta_{32}\end{pmatrix} & \begin{pmatrix}\beta_{21}\beta_{33}^{+}\\ \beta_{23}\beta_{31}\end{pmatrix} & \begin{pmatrix}\beta_{22}\beta_{31}^{+}\\ \beta_{21}\beta_{32}\end{pmatrix} \\ 2\beta_{31}\beta_{11} & 2\beta_{32}\beta_{12} & 2\beta_{33}\beta_{13} & \begin{pmatrix}\beta_{13}\beta_{32}^{+}\\ \beta_{12}\beta_{33}\end{pmatrix} & \begin{pmatrix}\beta_{13}\beta_{31}^{+}\\ \beta_{11}\beta_{13}\end{pmatrix} & \begin{pmatrix}\beta_{11}\beta_{32}^{+}\\ \beta_{12}\beta_{31}\end{pmatrix} \\ 2\beta_{11}\beta_{21} & 2\beta_{12}\beta_{22} & 2\beta_{13}\beta_{23} & \begin{pmatrix}\beta_{12}\beta_{23}^{+}\\ \beta_{13}\beta_{22}\end{pmatrix} & \begin{pmatrix}\beta_{13}\beta_{21}^{+}\\ \beta_{11}\beta_{23}\end{pmatrix} & \begin{pmatrix}\beta_{11}\beta_{22}^{+}\\ \beta_{12}\beta_{21}\end{pmatrix} \end{bmatrix} \quad (2)$$

An unambiguous method for determining the elements of γ will be given in the next section. This one array is the same (algebraically) for the calculation of all elastic constants, no matter what the crystal symmetry.

In the generalized form of Hooke's Law, the components of strain e_{xy} are written as linear functions of the components of stress X_{xy}, and the coefficients S_{ab} are defined to be the *elastic constants*. (Conversely, the stresses are linear functions of the strains and the coefficients C_{cd} are the *elastic moduli**.) Furthermore, from the conservation of energy, $S_{ab} = S_{ba}$ (and $C_{cd} = C_{dc}$) and the 36 elements connecting the six components of strain with the six components of stress are reduced to 21; we have then the following scheme:

	X_{xx}	X_{yy}	X_{zz}	X_{yz}	X_{zx}	X_{xy}
e_{xx}	S_{11}	S_{12}	S_{13}	S_{14}	S_{15}	S_{16}
e_{yy}	S_{12}	S_{22}	S_{23}	S_{24}	S_{25}	S_{26}
e_{zz}	S_{13}	S_{23}	S_{33}	S_{34}	S_{35}	S_{36}
e_{yz}	S_{14}	S_{24}	S_{34}	S_{44}	S_{45}	S_{46}
e_{zx}	S_{15}	S_{25}	S_{35}	S_{45}	S_{55}	S_{56}
e_{xy}	S_{16}	S_{26}	S_{36}	S_{46}	S_{56}	S_{66}

(3)

(Interchanging e_{xy} and X_{xy}, a similar array can be written for C_{cd}.)

The rows and columns of S and γ are denoted by running subscripts λ and ϱ respectively ($\lambda, \varrho = 1, 2, \ldots, 6$), i.e. $\gamma_{43} = 2\beta_{23}\beta_{33}$.

3. To obtain $S'_{\lambda\varrho}$, write the λ row of γ, the array of S, and the ϱ row of γ *written as a column*, as follows:

$$S'_{\lambda\varrho} = \begin{bmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \gamma_{\lambda1} & \gamma_{\lambda2} & \gamma_{\lambda3} & \gamma_{\lambda4} & \gamma_{\lambda5} & \gamma_{\lambda6} \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix} \begin{bmatrix} S_{11} & S_{12} & S_{13} & S_{14} & S_{15} & S_{16} \\ S_{12} & S_{22} & S_{23} & S_{24} & S_{25} & S_{26} \\ S_{13} & S_{23} & S_{33} & S_{34} & S_{35} & S_{36} \\ S_{14} & S_{24} & S_{34} & S_{44} & S_{45} & S_{46} \\ S_{15} & S_{25} & S_{35} & S_{45} & S_{55} & S_{56} \\ S_{16} & S_{26} & S_{36} & S_{46} & S_{56} & S_{66} \end{bmatrix} \begin{bmatrix} \cdot & \gamma_{\varrho1} & \cdot & \cdot & \cdot & \cdot \\ \cdot & \gamma_{\varrho2} & \cdot & \cdot & \cdot & \cdot \\ \cdot & \gamma_{\varrho3} & \cdot & \cdot & \cdot & \cdot \\ \cdot & \gamma_{\varrho4} & \cdot & \cdot & \cdot & \cdot \\ \cdot & \gamma_{\varrho5} & \cdot & \cdot & \cdot & \cdot \\ \cdot & \gamma_{\varrho6} & \cdot & \cdot & \cdot & \cdot \end{bmatrix} \quad (4)$$

4. Perform the following operations: Multiply the first row of S times the column $(\gamma_{\varrho1}, \ldots, \gamma_{\varrho6})$ term by term—$(S_{11}\gamma_{\varrho1}+S_{12}\gamma_{\varrho2}+\ldots+S_{16}\gamma_{\varrho6})$—and multiply this by the 1st element of the row, $\gamma_{\lambda1}$. Repeat for the second row of S and the second element of the row, $\gamma_{\lambda2}(S_{12}\gamma_{\varrho1}+\ldots+S_{26}\gamma_{\varrho6})$, etc. The sum of these six expressions is $S'_{\lambda\varrho}$. [$S'_{\lambda\varrho}$ will be recognized as the $\lambda\varrho$ element of the 'transformed' matrix S' and γ as the 'transformation matrix' in this special six-dimensional space. In § 3 it will be shown how (4) results from the simultaneous contraction of quadratic combinations of the direction cosines and a fourth rank tensor.]

Two examples will serve to illustrate the brevity and simplicity of this method: Suppose S'_{23} is required for the most general case of 21 elastic constants. The second and third rows of γ are substituted in (4) as a row and column respectively and the answer written immediately:

* These quantities are often called the coefficients of *compliance* and *elasticity* respectively, and to further confuse the issue, in some references (Wooster, 1938), the *C*'s are called the *elastic constants* and the *S*'s the *moduli*.

$$S'_{23} = \begin{bmatrix} . & . & . & . & . & . \\ \beta_{21}^2 & \beta_{22}^2 & \beta_{23}^2 & \beta_{22}\beta_{23} & \beta_{21}\beta_{23} & \beta_{21}\beta_{22} \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ . & . & . & . & . & . \end{bmatrix} \begin{bmatrix} S_{11} & S_{12} & S_{13} & S_{14} & S_{15} & S_{16} \\ S_{12} & S_{22} & S_{23} & S_{24} & S_{25} & S_{26} \\ S_{13} & S_{23} & S_{33} & S_{34} & S_{35} & S_{36} \\ S_{14} & S_{24} & S_{34} & S_{44} & S_{45} & S_{46} \\ S_{15} & S_{25} & S_{35} & S_{45} & S_{55} & S_{56} \\ S_{16} & S_{26} & S_{36} & S_{46} & S_{56} & S_{66} \end{bmatrix} \begin{bmatrix} . & . & \beta_{31}^2 & . & . & . \\ . & . & \beta_{32}^2 & . & . & . \\ . & . & \beta_{33}^2 & . & . & . \\ . & . & \beta_{32}\beta_{33} & . & . & . \\ . & . & \beta_{33}\beta_{31} & . & . & . \\ . & . & \beta_{31}\beta_{32} & . & . & . \end{bmatrix} \tag{5}$$

$$= \beta_{21}^2(S_{11}\beta_{31}^2+S_{12}\beta_{32}^2+S_{13}\beta_{33}^2+S_{14}\beta_{32}\beta_{33}+S_{15}\beta_{33}\beta_{31}+S_{16}\beta_{31}\beta_{32})+$$
$$\beta_{22}^2(S_{12}\beta_{31}^2+S_{22}\beta_{32}^2+S_{23}\beta_{33}^2+S_{24}\beta_{32}\beta_{33}+S_{25}\beta_{33}\beta_{31}+S_{26}\beta_{31}\beta_{32})+$$
$$(\ldots)+(\ldots)+(\ldots)+$$
$$\beta_{21}\beta_{22}(S_{16}\beta_{31}^2+S_{26}\beta_{32}^2+S_{36}\beta_{33}^2+S_{46}\beta_{32}\beta_{33}+S_{56}\beta_{33}\beta_{31}+S_{66}\beta_{31}\beta_{32}) .$$

After collecting the coefficients of each $S_{\delta\sigma}$, (5) is seen to be the same as the relation stated in the literature (Cady, 1946)*:

$$S'_{23} = \beta_{21}^2\beta_{31}^2S_{11}+\beta_{22}^2\beta_{32}^2S_{22}+\beta_{23}^2\beta_{33}^2S_{33}+(\beta_{22}^2\beta_{33}^2+\beta_{32}^2\beta_{23}^2)S_{23}+\ldots+\beta_{22}\beta_{32}\beta_{23}\beta_{33}S_{44}+\ldots$$
$$+\beta_{21}\beta_{31}(\beta_{22}\beta_{33}+\beta_{21}\beta_{32})S_{56}+(\beta_{21}^2\beta_{32}\beta_{33}+\beta_{31}^2\beta_{22}\beta_{33})S_{14}+\ldots$$
$$+\beta_{21}\beta_{31}(\beta_{21}\beta_{33}+\beta_{23}\beta_{31})S_{15}+\beta_{21}\beta_{31}(\beta_{21}\beta_{32}+\beta_{22}\beta_{31})S_{16}+\ldots .$$

If S'_{11} is required for a cubic crystal, the proper array of elastic constants for cubic symmetry and the first row of γ are inserted in (4) and the answer written:

$$S'_{11} = \begin{bmatrix} \beta_{11}^2 & \beta_{12}^2 & \beta_{13}^2 & \beta_{12}\beta_{13} & \beta_{13}\beta_{11} & \beta_{11}\beta_{12} \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ . & . & . & . & . & . \end{bmatrix} \begin{bmatrix} S_{11} & S_{12} & S_{12} & & & \\ S_{12} & S_{11} & S_{12} & & & \\ S_{12} & S_{12} & S_{11} & & & \\ & & & S_{44} & & \\ & & & & S_{44} & \\ & & & & & S_{44} \end{bmatrix} \begin{bmatrix} \beta_{11}^2 & . & . & . & . & . \\ \beta_{12}^2 & . & . & . & . & . \\ \beta_{13}^2 & . & . & . & . & . \\ \beta_{12}\beta_{13} & . & . & . & . & . \\ \beta_{13}\beta_{11} & . & . & . & . & . \\ \beta_{11}\beta_{12} & . & . & . & . & . \end{bmatrix} \tag{6}$$

$$= \beta_{11}(\beta_{11}S_{11}+\beta_{12}S_{12}+\beta_{13}S_{12})+\beta_{12}(\beta_{11}S_{12}+\beta_{12}S_{11}+\beta_{13}S_{12})+\ldots+\beta_{11}\beta_{12}(\beta_{12}\beta_{11}S_{44});$$
$$\text{i.e. } S'_{11} = S_{11}-\{2(S_{11}-S_{12})-S_{44}\}(\beta_{11}\beta_{12}+\beta_{11}\beta_{13}+\beta_{12}\beta_{13}) ,$$

which is the expected result (Zener, 1948).

(B) The elastic moduli

The moduli (the C's) are expressed in a rotated axis system using the same calculation except that the matrix γ is replaced by the matrix α†:

$$\alpha = \begin{bmatrix} \beta_{11}^2 & \beta_{12}^2 & \beta_{13}^2 & 2\beta_{12}\beta_{13} & 2\beta_{13}\beta_{11} & 2\beta_{11}\beta_{12} \\ \beta_{21}^2 & \beta_{22}^2 & \beta_{23}^2 & 2\beta_{22}\beta_{23} & 2\beta_{23}\beta_{21} & 2\beta_{21}\beta_{22} \\ \beta_{31}^2 & \beta_{32}^2 & \beta_{33}^2 & 2\beta_{32}\beta_{33} & 2\beta_{33}\beta_{31} & 2\beta_{31}\beta_{32} \\ \beta_{21}\beta_{31} & \beta_{22}\beta_{32} & \beta_{23}\beta_{33} & \begin{pmatrix}\beta_{22}\beta_{33}^+ \\ \beta_{23}\beta_{32}\end{pmatrix} & \begin{pmatrix}\beta_{21}\beta_{33}^+ \\ \beta_{23}\beta_{31}\end{pmatrix} & \begin{pmatrix}\beta_{22}\beta_{31}^+ \\ \beta_{21}\beta_{32}\end{pmatrix} \\ \beta_{31}\beta_{11} & \beta_{32}\beta_{12} & \beta_{33}\beta_{13} & \begin{pmatrix}\beta_{13}\beta_{32}^+ \\ \beta_{12}\beta_{33}\end{pmatrix} & \begin{pmatrix}\beta_{13}\beta_{31}^+ \\ \beta_{11}\beta_{33}\end{pmatrix} & \begin{pmatrix}\beta_{11}\beta_{32}^+ \\ \beta_{12}\beta_{31}\end{pmatrix} \\ \beta_{11}\beta_{21} & \beta_{12}\beta_{22} & \beta_{13}\beta_{23} & \begin{pmatrix}\beta_{12}\beta_{23}^+ \\ \beta_{13}\beta_{22}\end{pmatrix} & \begin{pmatrix}\beta_{13}\beta_{21}^+ \\ \beta_{11}\beta_{23}\end{pmatrix} & \begin{pmatrix}\beta_{11}\beta_{22}^+ \\ \beta_{12}\beta_{21}\end{pmatrix} \end{bmatrix} \tag{2'}$$

The sequence of operations delineated above for calculating the S'_{ab} are thus the same for C'_{cd} except that the rows and columns of γ and S are replaced by those of α and C. It can easily be verified that the C'_{cd} found in this way agree with those in the literature found by much more cumbersome methods (Cady, 1946). The connection between α and γ will be treated in § 3.

3. Mathematical development

The transformation between two sets of unitary orthogonal axes, (1), is written in the standard tensor notation as

$$x'_k = \beta_{ki}x_i . \tag{7}$$

The matrix of the stresses,

$$X = \begin{pmatrix} X_{xx} & X_{xy} & X_{xz} \\ X_{yx} & X_{yy} & X_{yz} \\ X_{zx} & X_{zy} & X_{zz} \end{pmatrix}, \tag{8}$$

becomes simply

$$\begin{pmatrix} X_{11} & X_{12} & X_{13} \\ X_{21} & X_{22} & X_{23} \\ X_{31} & X_{32} & X_{33} \end{pmatrix}$$

* An error in the coefficient of S_{16} in the expression for S'_{23} in this reference (equation (26), p. 70) has been corrected in this paper.

† It has been pointed out to the authors that the 6×6 array α has previously been reported by Bond (1943). However, it was arrived at by collecting the coefficients of the elastic constants in the rotated axis system and arranging them in an arbitrary scheme rather than by the tensor method herein presented.

and transforms as a second rank tensor:

$$X'_{rs} = \beta_{rm}\beta_{sn}X_{mn} . \tag{9}$$

Because of the conditions for equilibrium, X is symmetric, i.e.

$$X_{xy} = X_{yx} = X_{12} = X_{21} , \quad \text{etc.} \tag{10}$$

The strain matrix is also symmetric, but if e_{xx}, e_{xy}, etc. are defined as the strains in the usual manner, the strains do *not* transform as the elements of a second rank tensor (Mason, 1950). However, if we write the 'strain' tensor elements as

$$e = \begin{pmatrix} e_{xx} & \frac{1}{2}e_{xy} & \frac{1}{2}e_{xz} \\ \frac{1}{2}e_{xy} & e_{yy} & \frac{1}{2}e_{yz} \\ \frac{1}{2}e_{xz} & \frac{1}{2}e_{yz} & e_{zz} \end{pmatrix} = \begin{pmatrix} e_{11} & e_{12} & e_{13} \\ e_{12} & e_{22} & e_{23} \\ e_{13} & e_{23} & e_{33} \end{pmatrix}, \tag{11}$$

where $e_{11} = e_{xx}$, $e_{12} = \frac{1}{2}e_{xy}$, etc., then

$$e'_{ki} = \beta_{ko}\beta_{ip}e_{op} . \tag{12}$$

The two second rank tensors (8) and (11) are connected by a fourth rank tensor. One way in which the relationship between the tensor elements can be written is

$$e_{op} = s_{opmn}X_{mn} , \tag{13}$$

which again is Hooke's Law.

In a rotated axis system,

$$e'_{ki} = s'_{kirs}X'_{rs} , \tag{14}$$

and from (12)

$$e'_{ki} = \beta_{ko}\beta_{ip}e_{op} .$$

Substituting from (13),

$$e'_{ki} = \beta_{ko}\beta_{ip}s_{opmn}X_{mn} .$$

But from (9)

$$X_{mn} = \beta_{rm}\beta_{sn}X'_{rs} , \tag{15}$$

and hence

$$e'_{ki} = \beta_{ko}\beta_{ip}s_{opmn}\beta_{rm}\beta_{sn}X'_{rs} . \tag{16}$$

Thus, comparing (14) and (16),

$$s'_{kirs} = \beta_{ko}\beta_{ip}s_{opmn}\beta_{rm}\beta_{sn} . \tag{17}$$

Symmetry and energy-conservation considerations indicate that

$$s_{opmn}=s_{opmn}=s_{ponm}=s_{pomn}=s_{mnop}=s_{nmop}=s_{mnpo}=s_{nmpo} , \tag{18}$$

and the 81 s_{opmn} are reduced to 21. Thus (13) can be written in the form of the array:

	X_{11}	X_{22}	X_{33}	X_{23}	X_{31}	X_{12}
e_{11}	s_{1111}	s_{1122}	s_{1133}	$2s_{1123}$	$2s_{1131}$	$2s_{1112}$
e_{22}	s_{1122}	s_{2222}	s_{2233}	$2s_{2223}$	$2s_{2231}$	$2s_{2212}$
e_{33}	s_{1133}	s_{2233}	s_{3333}	$2s_{3323}$	$2s_{3331}$	$2s_{3312}$
e_{23}	s_{1123}	s_{2223}	s_{2333}	$2s_{2323}$	$2s_{2331}$	$2s_{2312}$
e_{31}	s_{1131}	s_{2231}	s_{3331}	$2s_{2331}$	$2s_{3131}$	$2s_{3112}$
e_{12}	s_{1112}	s_{2212}	s_{3312}	$2s_{2312}$	$2s_{3112}$	$2s_{1212}$

(19)

Comparing the s_{opmn} of (19) with the S_{ab} of (3), it is seen that

$$\left.\begin{array}{llll} s_{1111} = S_{11} & s_{1123} = \frac{1}{2}S_{14} & \text{etc.} \\ s_{1122} = S_{12} & s_{2323} = \frac{1}{4}S_{44} & \text{etc.} \\ s_{1133} = S_{13} & & \end{array}\right\} \tag{20}$$

Consideration of (18) and (20) leads immediately to the following contracting scheme (Wooster, 1938):

$$\left.\begin{array}{cccccccc} 11 & 22 & 33 & 23, & 31, & 12, & ki, op, & \text{etc.} \\ \downarrow & \downarrow & \downarrow & 32 & 13 & 21 & & \\ 1 & 2 & 3 & 4 & 5 & 6 & \delta, \sigma, \varrho & \text{etc.} \end{array}\right\} \tag{21}$$

The development thus far has been included to maintain a notation consistent with the literature and to serve as a point of departure for what follows.

The elastic constants are now required in the rotated (primed) axis system. Standard texts (Cady, 1946; Zener, 1948; Voigt, 1910*) usually suggest the following procedure: Let S'_{ab} be required, and use one of the equations connecting e'_{ki} and the X'_{rs} by a matrix of the S'_{ab} (similar to (3)). Assume a single stress component X'_{rs} be impressed, and write the six equations (15) in terms of it. The values are then substituted in (13), giving the e_{op} in terms of S_{cd}, β_{ko}, and X'_{rs}. The e_{op} are in turn substituted in (12). Then S'_{ab} is the coefficient of $X'_b = X'_{rs}$ (where b is the contraction of rs according to (21)) in the expression for $e'_a = e'_{ki}$, and in the general case has 21 terms.

Clearly this procedure is long and tedious. The introduction of the tensor notation permits a considerable reduction in the labor required and decreases the opportunity for errors, since the solution now involves the multiple summation indicated in (17) and the substitution given in (20). But even this is quite time-consuming unless the crystal possesses a high degree of symmetry.

However, even a greater simplification results, which permits problems of this type to be solved quickly and easily, if the s_{opmn} and the quadratic products of the β_{uv} are contracted *simultaneously* in the special way described below.

Suppose a particular S'_{ab} is desired (this corresponds to a particular $s'_{ikrs} = S'_{\lambda\varrho}$). Because both k and i are fixed in (17), it is seen that there are only nine quadratic products of $\beta_{ko}\beta_{ip}$ as o and p vary from 1 to 3. Furthermore, since $s_{opmn} = s_{pomn}$, terms $\beta_{kp}\beta_{io}$ and $\beta_{ko}\beta_{ip}$ $(o \neq p)$ can be combined and thus the nine terms are reduced to six for a given k and i. Hence these terms can be written

$$\beta_{ko}\beta_{ip} = \gamma_{\lambda\delta} , \tag{22}$$

* Voigt's treatment differs from that of Cady (1946) and Zener (1948) (and described in this paper) in that it involves setting up the strain energy function in the two coordinate systems, transforming the coordinates, and comparing the coefficients of the elastic constants. Like the treatments of Cady and Zener, it is quite complex and requires various mnemonic devices to obtain the proper coefficients which appear in the expressions, e.g. how to write S'_{23} once S'_{13} is obtained, etc..

where λ corresponds to the contraction of ko according to (21) in the special way defined by (22), and similarly for δ. This step, which defines $\gamma_{\lambda\delta}$ and forms the basis for this method, is seen more clearly by the following scheme:

$$\left.\begin{aligned} \beta_{k1}^2 &\equiv \gamma_{\lambda 1} \\ \beta_{k2}^2 &\equiv \gamma_{\lambda 2} \\ \beta_{k3}^2 &\equiv \gamma_{\lambda 3} \\ \beta_{k2}\beta_{k3} &\equiv \gamma_{\lambda 4} \\ \beta_{k3}\beta_{k1} &\equiv \gamma_{\lambda 5} \\ \beta_{k1}\beta_{k2} &\equiv \gamma_{\lambda 6} \end{aligned}\right\} \begin{matrix} k = i \\ \lambda = 1, 2, 3 \end{matrix}$$

$$\left.\begin{aligned} 2\beta_{k1}\beta_{i1} &\equiv \gamma_{\lambda 1} \\ 2\beta_{k2}\beta_{i2} &\equiv \gamma_{\lambda 2} \\ 2\beta_{k3}\beta_{i3} &\equiv \gamma_{\lambda 3} \\ (\beta_{k3}\beta_{i2}+\beta_{k2}\beta_{i3}) &\equiv \gamma_{\lambda 4} \\ (\beta_{k1}\beta_{i3}+\beta_{k3}\beta_{i1}) &\equiv \gamma_{\lambda 5} \\ (\beta_{k2}\beta_{i1}+\beta_{k1}\beta_{i2}) &\equiv \gamma_{\lambda 6} \end{aligned}\right\} \begin{matrix} k \neq i \\ \lambda = 4, 5, 6 \end{matrix} \qquad (23)$$

The reason for the discrepancy between the terms with $k = i$ and $k \neq i$ becomes apparent from consideration of (20).

With this effective collapsing of the β quadratic terms from nine to six, the S_{ab} of (3) are now the proper constants in our special method of summation, rather than the s_{opmn} of (19). This is seen by performing the sum in (17), collecting terms, using the relations of (20) and substituting (22). Thus, instead of using (17) etc., the S'_{ab} can be obtained directly as

$$S'_{\lambda\varrho} = \sum_{\delta=1}^{\delta=6} \sum_{\sigma=1}^{\sigma=6} \gamma_{\lambda\delta} S_{\delta\sigma} \gamma_{\varrho\sigma} \,. \qquad (24)$$

This is the $\lambda\varrho$ term of the 'transformed' matrix S', i.e.

$$S' = \gamma S \tilde{\gamma} \,, \qquad (25)$$

where γ is the matrix of the terms formed in accordance with (23) and is given in (2), S is the matrix of (3) and $\tilde{\gamma}$ is the transpose of γ formed by interchanging the rows and columns of (2). Hence, using the standard methods of matrix algebra and writing only those terms which contribute to $S'_{\lambda\varrho}$, (24) can be written as (4) and thus the method stated in § 2 has been proved.

Likewise, one could in a straightforward manner obtain the matrix α by writing instead of (13),

$$X_{op} = c_{opmn} e_{mn} \qquad (13')$$

and, proceeding in the same way, by simultaneous contraction obtain

$$C' = \alpha C \tilde{\alpha} \qquad (25')$$

and (2').

However, it is much easier (and more instructive) to obtain the relation between α and γ by considering some function of both the S's and the C's which is invariant under a transformation of axes. The simplest function of this type is the product of the two matrices S (3) and C (Zener, 1948). Since $X = Ce$ and $e = SX$, therefore $X = CSX$ and thus $CS = SC = I$, where I is the indentity matrix (with 1's along the main diagonal and zeros elsewhere). Thus S and C are reciprocally related:

$$S = C^{-1} \text{ (and } C = S^{-1}) \,, \qquad (26)$$

where C^{-1} is the reciprocal matrix of C, i.e. its ijth term is $C_{ij}^{-1} = C^{ji}(-1)^{i+j}/\Delta C$, where ΔC is the determinant of the matrix C, and C^{ji} is the cofactor formed by deleting the jth row and ith column of the determinant of C (Wills, 1946). I is invariant under a transformation of axes and thus, from (25) and (25'),

$$C'S' = I = \alpha C \tilde{\alpha} \gamma S \tilde{\gamma}, \quad \tilde{\alpha}\gamma = I = \alpha\tilde{\gamma}$$

and thus

$$\gamma = \tilde{\alpha}^{-1} \,, \qquad (27)$$

which can be verified termwise from (2) and (2').

Hence it is seen that α and γ are not independent* and thus, when one is determined, the other is known. Computations are further facilitated since both γ and α are unitary, i.e. $\Delta\alpha = \Delta\gamma = 1$.

4. Summary

A simple, easily remembered scheme is developed for transforming the elastic constants (or the elements of any fourth rank tensor† connecting two symmetric second rank tensor) from one rectangular coordinate system to another system rotated with respect to the first. The application of this method, instead of the conventional methods, reduces the number of steps to a minimum with a corresponding reduction in the chance for errors in the computation. The saving in time and labor is considerable, as is shown by two typical examples.

This work was sponsored in part by the Office of Ordinance Research, U.S. Army (Contract DA-30-069-ORD-459) under the supervision of Dr T. A. Read, whose suggestions regarding the presentation are appreciated.

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* Bond (1943) obtained (27) by considering the invariance of the strain energy, which of course cannot depend upon the reference system employed and is invariant under a transformation of axes.

† The fourth rank tensor, which can be reduced from 81 to 36 terms if it connects two symmetric second rank tensors, does not have to be symmetric itself for the formulae (18)–(23) to be correct. The method is applicable even if $S_{\lambda\sigma} \neq S_{\sigma\lambda}$ ($s_{opmn} \neq s_{mnop}$) since the development in no way depends upon the symmetry of S. In the case of elastic constants, $s_{opmn} = s_{opnm}$ because of the symmetry of e and X; $s_{opmn} = s_{mnop}$ because of conservation of energy, i.e. $\partial U/\partial e = X$, where U is the strain energy function.

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An X-ray Study of α-Keratin. I. A General Diffraction Theory for Convoluted Chain Structures and an Approximate Theory for Coiled-Coils

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(*Received* 10 *June* 1955)

A fibre structure is examined consisting of a periodic distribution of electron density along an infinite line which is folded or coiled in space in a pattern arbitrarily complex but repeating regularly along the fibre axis. The electron-density distribution on the spiral is expressed as a Fourier series, periodic in the distance measured along the line, and the same holds for each of the cartesian coordinates of a point of the spiral. The expression for the structure amplitude on any layer can be written as a product of Fourier coefficients of these four series. The approximate theory for the coiled coil regards the compound helix as a minor helix deformed with the periodicity of the major helix, the scattering contribution of each turn of the minor helix being thereby modulated in phase and amplitude. The diffraction pattern of a three-strand cable composed of α_1 helices has been calculated in the region of meridional spacing 6·1–4·7 Å and shows qualitative agreement with the observed porcupine-quill pattern.

Introduction

Pauling & Corey (1951*a*) proposed a structure for α-keratin consisting of α-helices packed together in alignment with the fibre axis, and Perutz (1951) pointed out that the observation of a relatively strong meridional 1·5 Å reflection in materials such as horse hair and porcupine quill gave strong support to this idea. On the other hand, the projection on the fibre axis of the electron density of the α-helix shows no periodicity corresponding to the helix repeat distance, and so the strong meridional arc at 5·18 Å, characteristic of the α-keratin pattern, cannot be explained by the simple model of α-helices in parallel array. The way out of this difficulty was shown in principle by Crick (1952) and Pauling & Corey (1953), who suggested that the α-helix axis was inclined to the fibre axis and itself followed a larger helix. It is easily seen that the projection on to the fibre axis of such a coiled-coil structure possesses a periodicity corresponding roughly to the α-helix repeat, and hence will give some approach to the observed meridional diffraction pattern. The apparently complex calculation of the diffraction pattern of a structure containing coiled-coils can be much simplified by regarding the structure as a grating composed of a repetition of single turns of the minor helix (i.e. the α-helix) with a superimposed modulation in scattering amplitude and phase, the modulation wavelength being the major helix axial-repeat distance. On this basis the writer has derived a simple approximate theory for the rapid calculation of the meridional and near-meridional diffraction pattern of coiled-coils assembled in multi-strand cables. An exact theory for the calculation of the whole diffraction pattern of coiled coils has been developed independently by Crick (1953*a*).

The present paper describes a general diffraction theory applicable to fibres consisting of atomic chains folded in arbitrarily complex fashion. This reduces to Crick's formula as a special case. An account is then given of the approximate theory. It is compared with the exact theory, and applied to calculate the diffrac-

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