International Tables for Crystallography (2006). Vol. D, Section 1.1.4.10.3, pp. 24–25.

(ii) Groups $m\bar{3}m$, 432, $\bar{4}3m$, and spherical system: the reduced tensors are already symmetric (see Sections 1.1.4.9.7 and 1.1.4.9.8).

1.1.4.10. *Reduced form of polar and axial tensors – matrix representation*

1.1.4.10.1. *Introduction*

Many tensors representing physical properties or physical quantities appear in relations involving symmetric tensors. Consider, for instance, the strain S_{ij} resulting from the application of an electric field **E** (the piezoelectric effect):

$$S_{ij} = d_{ijk} E_k + Q_{ijkl} E_k E_l, \qquad (1.1.4.4)$$

where the first-order terms d_{ijk} represent the components of the third-rank converse piezoelectric tensor and the second-order terms Q_{ijkl} represent the components of the fourth-rank electrostriction tensor. In a similar way, the direct piezoelectric effect corresponds to the appearance of an electric polarization **P** when a stress T_{jk} is applied to a crystal:

$$P_i = d_{ijk} T_{jk}. \qquad (1.1.4.5)$$

Owing to the symmetry properties of the strain and stress tensors (see Sections 1.3.1 and 1.3.2) and of the tensor product $E_k E_l$, there occurs a further reduction of the number of independent components of the tensors which are engaged in a contracted product with them, as is shown in Section 1.1.4.10.3 for third-rank tensors and in Section 1.1.4.10.5 for fourth-rank tensors.

1.1.4.10.2. *Stress and strain tensors – Voigt matrices*

The stress and strain tensors are symmetric because body torques and rotations are not taken into account, respectively (see Sections 1.3.1 and 1.3.2). Their components are usually represented using Voigt's one-index notation.

(i) Strain tensor

$$\left.\begin{array}{lll} S_1 = S_{11}; & S_2 = S_{22}; & S_3 = S_{33}; \\ S_4 = S_{23} + S_{32}; & S_5 = S_{31} + S_{13}; & S_6 = S_{12} + S_{21}; \\ S_4 = 2S_{23} = 2S_{32}; & S_5 = 2S_{31} = 2S_{13}; & S_6 = 2S_{12} = 2S_{21}. \end{array}\right\} \qquad (1.1.4.6)$$

The Voigt components S_α form a Voigt matrix:

$$\begin{pmatrix} S_1 & S_6 & S_5 \\ & S_2 & S_4 \\ & & S_3 \end{pmatrix}.$$

The terms of the leading diagonal represent the elongations (see Section 1.3.1). It is important to note that the non-diagonal terms, which represent the shears, are here equal to *twice* the corresponding components of the strain tensor. The components S_α of the Voigt strain matrix are therefore *not* the components of a tensor.

(ii) Stress tensor

$$\left.\begin{array}{lll} T_1 = T_{11}; & T_2 = T_{22}; & T_3 = T_{33}; \\ T_4 = T_{23} = T_{32}; & T_5 = T_{31} = T_{13}; & T_6 = T_{12} = T_{21}. \end{array}\right\}$$

The Voigt components T_α form a Voigt matrix:

$$\begin{pmatrix} T_1 & T_6 & T_5 \\ & T_2 & T_4 \\ & & T_3 \end{pmatrix}.$$

The terms of the leading diagonal correspond to principal normal constraints and the non-diagonal terms to shears (see Section 1.3.2).

1.1.4.10.3. *Reduction of the number of independent components of third-rank polar tensors due to the symmetry of the strain and stress tensors*

Equation (1.1.4.5) can be written

$$P_i = \sum_j d_{ijj} T_{jj} + \sum_{j\neq k} (d_{ijk} + d_{ikj}) T_{jk}.$$

The sums $(d_{ijk} + d_{ikj})$ for $j \neq k$ have a definite physical meaning, but it is impossible to devise an experiment that permits d_{ijk} and d_{ikj} to be measured separately. It is therefore usual to set them equal:

$$d_{ijk} = d_{ikj}. \qquad (1.1.4.7)$$

It was seen in Section 1.1.4.8.1 that the components of a third-rank tensor can be represented as a 9×3 matrix which can be subdivided into three 3×3 submatrices:

$$(\ \mathbf{1}\ |\ \mathbf{2}\ |\ \mathbf{3}\ ).$$

Relation (1.1.4.7) shows that submatrices **1** and **2** are identical. One puts, introducing a two-index notation,

$$\left.\begin{array}{rl} d_{ijj} = d_{i\alpha} & (\alpha = 1, 2, 3) \\ d_{ijk} + d_{ikj}\ (j \neq k) = d_{i\alpha} & (\alpha = 4, 5, 6). \end{array}\right\}$$

Relation (1.1.4.7) becomes

$$P_i = d_{i\alpha} T_\alpha.$$

The coefficients $d_{i\alpha}$ may be written as a 3×6 matrix:

$$\left(\begin{array}{ccc|ccc} 11 & 12 & 13 & 14 & 15 & 16 \\ 21 & 22 & 23 & 24 & 25 & 26 \\ 31 & 32 & 33 & 34 & 35 & 36 \end{array}\right).$$

This matrix is constituted by two 3×3 submatrices. The left-hand one is identical to the submatrix **1**, and the right-hand one is equal to the sum of the two submatrices **2** and **3**:

$$(\ \mathbf{1}\ |\ \mathbf{2} + \mathbf{3}\ ).$$

The inverse piezoelectric effect expresses the strain in a crystal submitted to an applied electric field:

$$S_{ij} = d_{ijk} E_k,$$

where the matrix associated with the coefficients d_{ijk} is a 9×3 matrix which is the transpose of that of the coefficients used in equation (1.1.4.5), as shown in Section 1.1.1.4.

The components of the Voigt strain matrix S_α are then given by

$$\left.\begin{array}{ll} S_\alpha = d_{iik} E_k & (\alpha = 1, 2, 3) \\ S_\alpha = S_{ij} + S_{ji} = (d_{ijk} + d_{jik}) E_k & (\alpha = 4, 5, 6). \end{array}\right\}$$

This relation can be written simply as

$$S_\alpha = d_{\alpha k} E_k,$$

where the matrix of the coefficients $d_{\alpha k}$ is a 6×3 matrix which is the transpose of the $d_{i\alpha}$ matrix.

There is another set of piezoelectric constants (see Section 1.1.5) which relates the stress, T_{ij}, and the electric field, E_k, which are both intensive parameters:

$$T_{ij} = e_{ijk} E_k, \qquad (1.1.4.8)$$

where a new piezoelectric tensor is introduced, e_{ijk}. Its components can be represented as a 3×9 matrix:

$$\begin{pmatrix} \mathbf{1} \\ \hline \mathbf{2} \\ \hline \mathbf{3} \end{pmatrix}.$$

Both sides of relation (1.1.4.8) remain unchanged if the indices i and j are interchanged, on account of the symmetry of the stress tensor. This shows that

$$e_{ijk} = e_{jik}.$$

Submatrices **2** and **3** are equal. One introduces here a two-index notation through the relation $e_{\alpha k} = e_{ijk}$, and the $e_{\alpha k}$ matrix can be written

$$\left(\frac{\mathbf{1}}{\mathbf{2}+\mathbf{3}}\right).$$

The relation between the full and the reduced matrix is therefore different for the d_{ijk} and the e_{kij} tensors. This is due to the particular property of the strain Voigt matrix (1.1.4.6), and as a consequence the relations between nonzero components of the reduced matrices are different for certain point groups (3, 32, 3m, $\bar{6}$, $\bar{6}2m$).

1.1.4.10.4. *Independent components of the matrix associated with a third-rank polar tensor according to the following point groups*

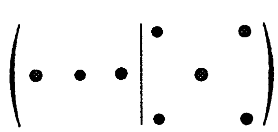
1.1.4.10.4.1. *Triclinic system*

(i) Group 1: all the components are independent. There are 18 components.

(ii) Group $\bar{1}$: all the components are equal to zero.

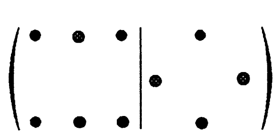
1.1.4.10.4.2. *Monoclinic system*

(i) Group 2: twofold axis parallel to Ox_2:



There are 8 independent components.

(ii) Group m:

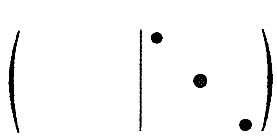


There are 10 independent components.

(iii) Group $2/m$: all the components are equal to zero.

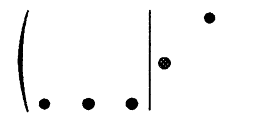
1.1.4.10.4.3. *Orthorhombic system*

(i) Group 222:



There are 3 independent components.

(ii) Group $mm2$:

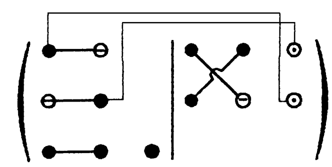


There are 5 independent components.

(iii) Group mmm: all the components are equal to zero.

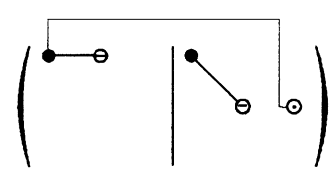
1.1.4.10.4.4. *Trigonal system*

(i) Group 3:



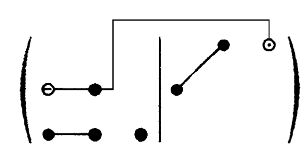
where the symbol ⊖ means that the corresponding component is equal to the opposite of that to which it is linked, ⊙ means that the component is equal to twice minus the value of the component to which it is linked for d_{ijk} and to minus the value of the component to which it is linked for e_{ijk}. There are 6 independent components.

(ii) Group 32, twofold axis parallel to Ox_1:



with the same conventions. There are 4 independent components.

(iii) Group 3m, mirror perpendicular to Ox_1:

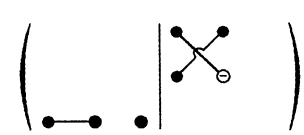


with the same conventions. There are 4 independent components.

(iv) Groups $\bar{3}$ and $\bar{3}m$: all the components are equal to zero.

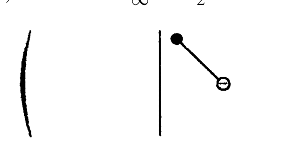
1.1.4.10.4.5. *Tetragonal, hexagonal and cylindrical systems*

(i) Groups 4, 6 and A_∞:



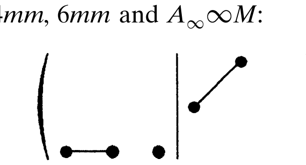
There are 4 independent components.

(ii) Groups 422, 622 and $A_\infty \infty A_2$:



There is 1 independent component.

(iii) Groups 4mm, 6mm and $A_\infty \infty M$:



There are 3 independent components.

references