International Tables for Crystallography (2006). Vol. D, Section 1.1.4.6.2, pp. 15–16.

$$A = B^T = B^{-1}.$$

Since the tensor is invariant under the action of the symmetry operator A, one has, according to Neumann's principle,

$$t'^{\alpha\beta}_{\gamma\delta} = t^{\alpha\beta}_{\gamma\delta}$$

and, therefore,

$$t^{\alpha\beta}_{\gamma\delta} = t^{ij}_{kl} A^\alpha_i A^\beta_j B^k_\gamma B^l_\delta. \qquad (1.1.4.1)$$

There are therefore a certain number of linear relations between the components of the tensor and the number of independent components is reduced. If there are p components and q relations between the components, there are $p - q$ independent components. This number is *independent* of the system of axes. When applied to each of the 32 point groups, this reduction enables one to find the form of the tensor in each case. It depends on the rank of the tensor. In the present chapter, the reduction will be derived for tensors up to the fourth rank and for all crystallographic groups as well as for the isotropic groups. An orthonormal frame will be assumed in all cases, so that co- and contravariance will not be apparent and the positions of indices as subscripts or superscripts will not be meaningful. The Ox_3 axis will be chosen parallel to the threefold, fourfold or sixfold axis in the trigonal, tetragonal and hexagonal systems. The accompanying software to the present volume enables the reduction for tensors of any rank to be derived.

1.1.4.6.2. *The operator A is in diagonal form*

1.1.4.6.2.1. *Introduction*

If one takes as the system of axes the eigenvectors of the operator A, the matrix is written in the form

$$\begin{pmatrix} \exp i\theta & 0 & 0 \\ 0 & \exp -i\theta & 0 \\ 0 & 0 & \pm 1 \end{pmatrix},$$

where θ is the rotation angle, Ox_3 is taken parallel to the rotation axis and coefficient A_3 is equal to +1 or −1 depending on whether the rotation axis is direct or inverse (proper or improper operator).

The equations (1.1.4.1) can then be simplified and reduce to

$$t^{ij}_{kl} = t^{ij}_{kl} A^\alpha_i A^\beta_j B^k_\gamma B^l_\delta \qquad (1.1.4.2)$$

(*without* any summation).

If the product $A^i_i A^j_j B^k_k B^l_l$ (without summation) is equal to unity, equation (1.1.4.2) is trivial and there is significance in the component t_{kl}. On the contrary, if it is different from 1, the only solution for (1.1.4.2) is that $t^{ij}_{kl} = 0$. One then finds immediately that certain components of the tensor are zero and that others are unchanged.

1.1.4.6.2.2. *Case of a centre of symmetry*

All the diagonal components are in this case equal to −1. One thus has:

(i) *Tensors of even rank*, $t^{ij\ldots} = (-1)^{2p} t^{ij\ldots}$. The components are not affected by the presence of the centre of symmetry. The reduction of tensors of even rank is therefore the same in a centred group and in its noncentred subgroups, that is in any of the 11 *Laue classes*:

$\bar{\mathbf{1}}$ 1
$\mathbf{2/m}$ 2, m
$\boldsymbol{mmm}$ 222, $2mm$
$\bar{\mathbf{3}}$ 3
$\bar{\mathbf{3}}\boldsymbol{m}$ 32, $3m$
$\mathbf{4/m}$ $\bar{4}$, 4
$\mathbf{4/mm}$ $\bar{4}2m$, 422, $4mm$
$\mathbf{6/m}$ $\bar{6}$, 6
$\mathbf{6/mm}$ $\bar{6}2m$, 622, $6mm$
$\boldsymbol{m}\bar{\mathbf{3}}$ 23
$\boldsymbol{m}\bar{\mathbf{3}}\boldsymbol{m}$ 432, $\bar{4}32$.

If a tensor is invariant with respect to two elements of symmetry, it is invariant with respect to their product. It is then sufficient to make the reduction for the generating elements of the group and (since this concerns a tensor of even rank) for the 11 *Laue classes*.

(ii) *Tensors of odd rank*, $t^{ij\ldots} = (-1)^{2p+1} t^{ij\ldots}$. *All* the components are equal to zero. The physical properties represented by tensors of rank 3, such as piezoelectricity, piezomagnetism, nonlinear optics, for instance, will therefore not be present in a centrosymmetric crystal.

1.1.4.6.2.3. *General case*

By replacing the matrix coefficients A^i_i by their expression, (1.1.4.2) becomes, for a proper rotation,

$$t^{jk\ldots} = t^{jk\ldots} \exp(ir\theta)\exp(-is\theta)(1)^t = t^{jk\ldots} \exp i(r-s)\theta,$$

where r is the number of indices equal to 1, s is the number of indices equal to 2, t is the number of indices equal to 3 and $r + s + t = p$ is the rank of the tensor. The component $t^{jk\ldots}$ is not affected by the symmetry operation if

$$(r - s)\theta = 2K\pi,$$

where K is an integer, and is equal to zero if

$$(r - s)\theta \neq 2K\pi.$$

The angle of rotation θ can be put into the form $2\pi/q$, where q is the order of the axis. The condition for the component not to be zero is then

$$r - s = Kq.$$

The condition is fulfilled differently depending on the rank of the tensor, p, and the order of the axis, q. Indeed, we have $r - s \le p$ and

$p = 2, r - s \le 2$: *the result of the reduction will be the same for any* $q \ge 3$;

$p = 3, r - s \le 3$: *the result of the reduction will be the same for any* $q \ge 4$;

$p = 4, r - s \le 4$: *the result of the reduction will be the same for any* $q \ge 5$.

It follows that:

(i) for tensors of rank 2, the reduction will be the same for trigonal (threefold axis), tetragonal (fourfold axis) and hexagonal (sixfold axis) groups;

(ii) for tensors of rank 3, the reduction will be the same for tetragonal and hexagonal groups;

(iii) for tensors of rank 4, the reduction will be different for trigonal, tetragonal and hexagonal groups.

The inconvenience of the diagonalization method is that the vectors and eigenvalues are, in general, complex, so in practice one uses another method. For instance, we may note that equation (1.1.4.1) can be written in the case of $p = 2$ by associating with the tensor a 3 × 3 matrix T:

$$T = BTB^T,$$

where B is the symmetry operation. Through identification of homologous coefficients in matrices T and BTB^T, one obtains relations between components t_{ij} that enable the determination of the independent components.

1.1.4.6.3. *The method of direct inspection*

The method of 'direct inspection', due to Fumi (1952*a*,*b*, 1987), is very simple. It is based on the fundamental properties of tensors; the components transform under a change of basis like a product of vector components (Section 1.1.3.2).

Examples

(1) Let us consider a tensor of rank 3 invariant with respect to a twofold axis parallel to Ox_3. The matrix representing this operator is

$$\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

The component t_{ijk} behaves under a change of axes like the product of the components x_i, x_j, x_k. The components x_1, x_2, x_3 of a vector become, respectively, $-x_1$, $-x_2$, x_3. To simplify the notation, we shall denote the components of the tensor simply by ijk. If, amongst the indices i, j and k, there is an even number (*including the number zero*) of indices that are equal to 3, the product $x_i x_j x_k$ will become $-x_i x_j x_k$ under the rotation. As the component 'ijk' remains invariant and is also equal to its opposite, it must be zero. 14 components will thus be equal to zero:

111, 122, 133, 211, 222, 133, 112, 121, 212, 221, 323, 331, 332, 313.

(2) Let us now consider that the same tensor of rank 3 is invariant with respect to a fourfold axis parallel to Ox_3. The matrix representing this operator and its action on a vector of coordinates x_1, x_2, x_3 is given by

$$\begin{pmatrix} x_2 \\ -x_1 \\ x_3 \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}. \qquad (1.1.4.3)$$

Coordinate x_1 becomes x_2, x_2 becomes $-x_1$ and x_3 becomes x_3. Component ijk transforms like product $x^i x^j x^k$ according to the rule given above. Since the twofold axis parallel to Ox_3 is a subgroup of the fourfold axis, we can start from the corresponding reduction. We find

$$\begin{array}{rcrcrcr} 311 & \Longleftrightarrow & 322 & : & t_{311} = & t_{322} \\ 123 & \Longleftrightarrow & -(213) & : & t_{123} = & -t_{213} \\ 113 & \Longleftrightarrow & 223 & : & t_{113} = & t_{223} \\ 333 & \Longleftrightarrow & 333 & : & t_{333} = & t_{333} \\ 132 & \Longleftrightarrow & -(231) & : & t_{132} = & -t_{231} \\ 131 & \Longleftrightarrow & 232 & : & t_{131} = & t_{232} \\ 312 & \Longleftrightarrow & -(321) & : & t_{312} = & -t_{321}. \end{array}$$

All the other components are equal to zero.

It is not possible to apply the method of direct inspection for point group 3. One must in this case use the matrix method described in Section 1.1.4.6.2; once this result is assumed, the method can be applied to all other point groups.

1.1.4.7. *Reduction of the components of a tensor of rank 2*

The reduction is given for each of the 11 Laue classes.

1.1.4.7.1. *Triclinic system*

Groups $\bar{1}$, 1: no reduction, the tensor has 9 independent components. The result is represented in the following symbolic way (Nye, 1957, 1985):

$$\begin{pmatrix} \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet \end{pmatrix}$$

where the sign $\bullet$ represents a nonzero component.

1.1.4.7.2. *Monoclinic system*

Groups $2m$, 2, m: it is sufficient to consider the twofold axis or the mirror. As the representative matrix is diagonal, the calculation is immediate. Taking the twofold axis to be parallel to Ox_3, one has

$$t_3^1 = t_1^3 = t_3^2 = t_2^3 = 0.$$

The other components are not affected. The result is represented as

$$\begin{pmatrix} \bullet & \bullet & \\ \bullet & \bullet & \\ & & \bullet \end{pmatrix}$$

There are 5 independent components. If the twofold axis is taken along axis Ox_2, which is the usual case in crystallography, the table of independent components becomes

$$\begin{pmatrix} \bullet & & \bullet \\ & \bullet & \\ \bullet & & \bullet \end{pmatrix}$$

1.1.4.7.3. *Orthorhombic system*

Groups mmm, $2mm$, 222: the reduction is obtained by considering two perpendicular twofold axes, parallel to Ox_3 and to Ox_2, respectively. One obtains

$$\begin{pmatrix} \bullet & & \\ & \bullet & \\ & & \bullet \end{pmatrix}$$

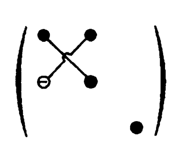
There are 3 independent components.

1.1.4.7.4. *Trigonal, tetragonal, hexagonal and cylindrical systems*

We remarked in Section 1.1.4.6.2.3 that, in the case of tensors of rank 2, the reduction is the same for threefold, fourfold or sixfold axes. It suffices therefore to perform the reduction for the tetragonal groups. That for the other systems follows automatically.

1.1.4.7.4.1. *Groups* $\bar{3}$, 3; $4/m$, $\bar{4}$, 4; $6/m$, $\bar{6}$, 6; $(A_\infty/M)C$, A_∞

If we consider a fourfold axis parallel to Ox_3 represented by the matrix given in (1.1.4.3), by applying the direct inspection method one finds



where the symbol $\ominus$ means that the corresponding component is numerically equal to that to which it is linked, but of opposite sign. There are 3 independent components.