International Tables for Crystallography (2006). Vol. D, Section 1.1.4.6, pp. 14–16.

1.1.4.5.3.2. *Tensors of higher rank*

If the rank of the tensor is higher than 2, the tensor may be antisymmetric with respect to the indices of one or several couples of indices.

(i) *Tensors of rank 3 antisymmetric with respect to every couple of indices*. A trilinear form $T(\mathbf{x},\mathbf{y},\mathbf{z}) = t_{ijk}x^i y^j z^k$ is said to be antisymmetric if it satifies the relations

$$\left.\begin{aligned} T(\mathbf{x},\mathbf{y},\mathbf{z}) &= -T(\mathbf{y},\mathbf{x},\mathbf{z})\\ &= -T(\mathbf{x},\mathbf{z},\mathbf{y})\\ &= -T(\mathbf{z},\mathbf{y},\mathbf{x}).\end{aligned}\right\}$$

Tensor t_{ijk} has 27 components. It is found that all of them are equal to zero, except

$$t_{123} = t_{231} = t_{312} = -t_{213} = -t_{132} = -t_{321}.$$

The three-times contracted product with the permutations tensor (Section 1.1.3.7.2), $(1/6)\varepsilon_{ijk}t_{ijk}$, is a *pseudoscalar* or *axial* scalar. It is not a usual scalar: the sign of this product changes when one changes the hand of the reference axes, change of basis represented by the matrix

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

Form $T(\mathbf{x},\mathbf{y},\mathbf{z})$ can also be written

$$T(\mathbf{x},\mathbf{y},\mathbf{z}) = Pt_{123},$$

where

$$P = \varepsilon_{ijk}x^i y^j z^k = \begin{vmatrix} x^1 & x^2 & x^3\\ y^1 & y^2 & y^3\\ z^1 & z^2 & z^3\end{vmatrix}$$

is the triple scalar product of the three vectors $\mathbf{x}$, $\mathbf{y}$, $\mathbf{z}$:

$$P = (\mathbf{x},\mathbf{y},\mathbf{z}) = (\mathbf{x}\wedge\mathbf{y}\cdot\mathbf{z}).$$

It is also a pseudoscalar. The permutation tensor is not a real tensor of rank 3: if the hand of the axes is changed, the sign of P also changes; P is therefore not a trilinear form.

Another example of a pseudoscalar is given by the rotatory power of an optically active medium, which is expressed through the relation (see Section 1.6.5.4)

$$\theta = \rho d,$$

where θ is the rotation angle of the light wave, d the distance traversed in the material and ρ is a pseudoscalar: if one takes the mirror image of this medium, the sign of the rotation of the light wave also changes.

(ii) *Tensor of rank 3 antisymmetric with respect to one couple of indices*. Let us consider a trilinear form such that

$$T(\mathbf{x},\mathbf{y},\mathbf{z}) = -T(\mathbf{y},\mathbf{x},\mathbf{z}).$$

Its components satisfy the relation

$$t^{iil} = 0; \quad t^{ijl} = -t^{jil}.$$

The twice contracted product

$$t_k^l = \tfrac{1}{2}\varepsilon_{ijk}t^{ijl}$$

is an *axial* tensor of rank 2 whose components are the independent components of the antisymmetric tensor of rank 3, t^{ijl}.

Examples

(1) *Hall constant*. The Hall effect is observed in semiconductors. If one takes a semiconductor crystal and applies a magnetic induction $\mathbf{B}$ and at the same time imposes a current density $\mathbf{j}$ at right angles to it, one observes an electric field $\mathbf{E}$ at right angles to the other two fields (see Section 1.8.3.4). The expression for the field can be written

$$E_i = R_{H\,ikl}j_k B_l,$$

where $R_{H\,ikl}$ is the Hall constant, which is a tensor of rank 3. However, because the direction of the current density is imposed by the physical law (the set of vectors $\mathbf{B}$, $\mathbf{j}$, $\mathbf{E}$ constitutes a right-handed frame), one has

$$R_{H\,ikl} = -R_{H\,kil},$$

which shows that $R_{H\,ikl}$ is an antisymmetric (axial) tensor of rank 3. As can be seen from its physical properties, only the components such that $i \neq k \neq l$ are different from zero. These are

$$R_{H\,123} = -R_{H\,213}; \quad R_{H\,132} = -R_{H\,312}; \quad R_{H\,312}; \quad R_{H\,321}.$$

(2) *Optical rotation*. The gyration tensor used to describe the property of optical rotation presented by gyrotropic materials (see Section 1.6.5.4) is an axial tensor of rank 2, which is actually an antisymmetric tensor of rank 3.

(3) *Acoustic activity*. The acoustic gyrotropic tensor describes the rotation of the polarization plane of a transverse acoustic wave propagating along the acoustic axis (see for instance Kumaraswamy & Krishnamurthy, 1980). The elastic constants may be expanded as

$$c_{ijkl}(\omega,\mathbf{k}) = c_{ijkl}(\omega) + \mathrm{i}d_{ijklm}(\omega)k_m + \ldots,$$

where d_{ijklm} is a fifth-rank tensor. Time-reversal invariance requires that $d_{ijklm} = -d_{jiklm}$, which shows that it is an antisymmetric (axial) tensor.

1.1.4.5.3.3. *Properties of axial tensors*

The two preceding sections have shown examples of axial tensors of ranks 0 (pseudoscalar), 1 (pseudovector) and 2. They have in common that all their components change sign when the sign of the basis is changed, and this can be taken as the definition of an axial tensor. Their components are the components of an antisymmetric tensor of higher rank. It is important to bear in mind that in order to obtain their behaviour in a change of basis, one should first determine the behaviour of the components of this antisymmetric tensor.

1.1.4.6. *Symmetry of tensors imposed by the crystalline medium*

Many papers have been devoted to the derivation of the invariant components of physical property tensors under the influence of the symmetry elements of the crystallographic point groups: see, for instance, Fumi (1951, 1952*a*,*b*,*c*, 1987), Fumi & Ripamonti (1980*a*,*b*), Nowick (1995), Nye (1957, 1985), Sands (1995), Sirotin & Shaskol'skaya (1982), and Wooster (1973). There are three main methods for this derivation: the matrix method (described in Section 1.1.4.6.1), the direct inspection method (described in Section 1.1.4.6.3) and the group-theoretical method (described in Section 1.2.4 and used in the accompanying software, see Section 1.2.7.4).

1.1.4.6.1. *Matrix method – application of Neumann's principle*

An operation of symmetry turns back the crystalline edifice on itself; it allows the physical properties of the crystal and the tensors representing them to be invariant. An operation of symmetry is equivalent to a change of coordinate system. In a change of system, a tensor becomes

$$t'^{\alpha\beta}_{\gamma\delta} = t^{ij}_{kl}A^\alpha_i A^\beta_j B^k_\gamma B^l_\delta.$$

If A represents a symmetry operation, it is a unitary matrix:

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

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
$\mathbf{mmm}$ 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 $r - s \leq p$ and

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

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

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

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

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

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

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

All the other components are equal to zero.

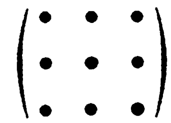
It is not possible to apply the method of direct inspection for point group 3. One must in this case use the matrix method described in Section 1.1.4.6.2; once this result is assumed, the method can be applied to all other point groups.

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):



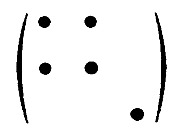
where the sign • represents a nonzero component.

1.1.4.7.2. *Monoclinic system*

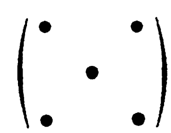
Groups $2m$, 2, m: it is sufficient to consider the twofold axis or the mirror. As the representative matrix is diagonal, the calculation is immediate. Taking the twofold axis to be parallel to Ox_3, one has

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

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

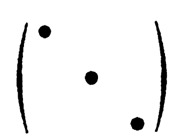


There are 5 independent components. If the twofold axis is taken along axis Ox_2, which is the usual case in crystallography, the table of independent components becomes



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



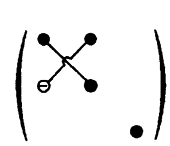
There are 3 independent components.

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 ⊖ means that the corresponding component is numerically equal to that to which it is linked, but of opposite sign. There are 3 independent components.