1.1. INTRODUCTION TO THE PROPERTIES OF TENSORS

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

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*, $t^{ij\cdots} = (-1)^{2p}t^{ij\cdots}$. 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*:

$\bar{1}$	1
$2/m$	2, m
mmm	222, $2mm$
$\bar{3}$	3
$\bar{3}m$	32, $3m$
$4/m$	$\bar{4}$, 4
$4/mm$	$\bar{4}2m$, 422, $4mm$
$6/m$	$\bar{6}$, 6
$6/mm$	$\bar{6}2m$, 622, $6mm$
$m\bar{3}$	23
$m\bar{3}m$	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*, $t^{ij\cdots} = (-1)^{2p+1}t^{ij\cdots}$. *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,

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

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 $t^{jk\cdots}$ 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:

$$T = BTB^T,$$