International Tables for Crystallography (2006). Vol. D, Section 1.1.4.7.3, p. 16.

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 $x_ix_jx_k$ will become $-x_ix_jx_k$ 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 $x^ix^jx^k$ 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

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

All the other components are equal to zero.

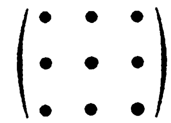
It is not possible to apply the method of direct inspection for point group 3. One must in this case use the matrix method described in Section 1.1.4.6.2; once this result is assumed, the method can be applied to all other point groups.

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):



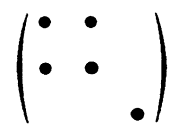
where the sign • represents a nonzero component.

1.1.4.7.2. *Monoclinic system*

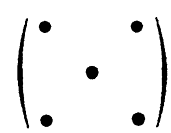
Groups $2m$, 2, m: it is sufficient to consider the twofold axis or the mirror. As the representative matrix is diagonal, the calculation is immediate. Taking the twofold axis to be parallel to Ox_3, one has

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

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

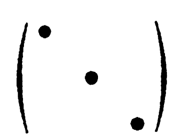


There are 5 independent components. If the twofold axis is taken along axis Ox_2, which is the usual case in crystallography, the table of independent components becomes



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



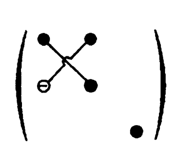
There are 3 independent components.

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.

  references