International Tables for Crystallography (2006). Vol. D, Section 1.1.4.5.3.3, p. 14.

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

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

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:

