

1.1. INTRODUCTION TO THE PROPERTIES OF TENSORS

$$\frac{A_\infty \infty A_2}{M \infty M} C \cap A_3 3A_2 \leq A_\infty \infty M.$$

If the applied compression is parallel to the threefold axis, the intersection is identical to the symmetry of the crystal,  $A_3 3A_2$ , which possesses symmetry elements that do not exist in the effect, and piezoelectricity cannot appear. This is of course obvious because the threefold axis is not polar. For all other directions, piezoelectricity may appear.

1.1.4.5. Intrinsic symmetry of tensors

1.1.4.5.1. Introduction

The symmetry of a tensor representing a physical property or a physical quantity may be due either to its own nature or to the symmetry of the medium. The former case is called intrinsic symmetry. It is a property that can be exhibited both by physical property tensors or by field tensors. The latter case is the consequence of Neumann’s principle and will be discussed in Section 1.1.4.6. It applies to physical property tensors.

1.1.4.5.2. Symmetric tensors

1.1.4.5.2.1. Tensors of rank 2

A bilinear form is symmetric if

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

Its components satisfy the relations

$$t_{ij} = t_{ji}.$$

The associated matrix,  $T$ , is therefore equal to its transpose  $T^T$ :

$$T = \begin{pmatrix} t_{11} & t_{12} & t_{13} \\ t_{21} & t_{22} & t_{23} \\ t_{31} & t_{32} & t_{33} \end{pmatrix} = T^T = \begin{pmatrix} t_{11} & t_{21} & t_{31} \\ t_{12} & t_{22} & t_{32} \\ t_{13} & t_{23} & t_{33} \end{pmatrix}.$$

In a space with  $n$  dimensions, the number of independent components is equal to

$$(n^2 - n)/2 + n = (n^2 + n)/2.$$

Examples

(1) The metric tensor (Section 1.1.2.2) is symmetric because the scalar product is commutative.

(2) The tensors representing one of the physical properties associated with the leading diagonal of the matrix of physical properties (Section 1.1.1.4), such as the dielectric constant. Let us take up again the demonstration of this case and consider a capacitor being charged. The variation of the stored energy per unit volume for a variation  $d\mathbf{D}$  of the displacement is

$$dW = \mathbf{E} \cdot d\mathbf{D},$$

where [equation (1.1.3.3)]

$$D^i = \varepsilon_j^i E^j.$$

Since both  $D^i$  and  $E^j$  are expressed through contravariant components, the expression for the energy should be written

$$dW = g_{ij} E^j dD^i.$$

If we replace  $D^i$  by its expression, we obtain

$$dW = g_{ij} \varepsilon_k^i E^j dE^k = \varepsilon_{jk} E^j dE^k,$$

where we have introduced the doubly covariant form of the dielectric constant tensor,  $\varepsilon_{jk}$ . Differentiating twice gives

$$\frac{\partial^2 W}{\partial E^k \partial E^j} = \varepsilon_{jk}.$$

If one can assume, as one usually does in physics, that the energy is a ‘good’ function and that the order of the derivatives is of little importance, then one can write

$$\frac{\partial^2 W}{\partial E^k \partial E^j} = \frac{\partial^2 W}{\partial E^j \partial E^k}.$$

As one can exchange the role of the dummy indices, one has

$$\partial^2 W / (\partial E^j \partial E^k) = \varepsilon_{kj}.$$

Hence one deduces that

$$\varepsilon_{jk} = \varepsilon_{kj}.$$

The dielectric constant tensor is therefore symmetric. One notes that the symmetry is conveyed on two indices of the same variance. One could show in a similar way that the tensor representing magnetic susceptibility is symmetric.

(3) There are other possible causes for the symmetry of a tensor of rank 2. The strain tensor (Section 1.3.1), which is a field tensor, is symmetric because one does not take into account the rotative part of the deformation; the stress tensor, also a field tensor (Section 1.3.1), is symmetric because one neglects body torques (couples per unit volume); the thermal conductivity tensor is symmetric because circulating flows do not produce any detectable effects *etc.*

1.1.4.5.2.2. Tensors of higher rank

A tensor of rank higher than 2 may be symmetric with respect to the indices of one or more couples of indices. For instance, by its very nature, the demonstration given in Section 1.1.1.4 shows that the tensors representing principal physical properties are of even rank. If  $n$  is the rank of the associated square matrix, the number of independent components is equal to  $(n^2 + n)/2$ . In the case of a tensor of rank 4, such as the tensor of elastic constants relating the strain and stress tensors (Section 1.3.3.2.1), the number of components of the tensor is  $3^4 = 81$ . The associated matrix is a  $9 \times 9$  one, and the number of independent components is equal to 45.

1.1.4.5.3. Antisymmetric tensors – axial tensors

1.1.4.5.3.1. Tensors of rank 2

A bilinear form is said to be antisymmetric if

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

Its components satisfy the relations

$$t_{ij} = -t_{ji}.$$

The associated matrix,  $T$ , is therefore also antisymmetric:

$$T = -T^T = \begin{pmatrix} 0 & t_{12} & t_{13} \\ -t_{12} & 0 & t_{23} \\ -t_{13} & -t_{23} & 0 \end{pmatrix}.$$

The number of independent components is equal to  $(n^2 - n)/2$ , where  $n$  is the number of dimensions of the space. It is equal to 3 in a three-dimensional space, and one can consider these components as those of a *pseudovector* or *axial* vector. It must never be forgotten that under a change of basis the components of an axial vector transform like those of a tensor of rank 2.

Every tensor can be decomposed into the sum of two tensors, one symmetric and the other one antisymmetric:

$$T = S + A,$$

with  $S = (T + T^T)/2$  and  $A = (T - T^T)/2$ .

## 1. TENSORIAL ASPECTS OF PHYSICAL PROPERTIES

*Example.* As shown in Section 1.1.3.7.2, the components of the vector product of two vectors,  $\mathbf{x}$  and  $\mathbf{y}$ ,

$$z_k = \varepsilon_{ijk} x^i y^j,$$

are really the independent components of an antisymmetric tensor of rank 2. The magnetic quantities,  $\mathbf{B}$ ,  $\mathbf{H}$  (Section 1.1.4.3.2), the tensor representing the pyromagnetic effect (Section 1.1.1.3) etc. are axial tensors.

### 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 satisfies 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

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

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  $\theta$  is the rotation angle of the light wave,  $d$  the distance traversed in the material and  $\rho$  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

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

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

$$c_{ijkl}(\omega, \mathbf{k}) = c_{ijkl}(\omega) + id_{ijklm}(\omega)k_m + \dots,$$

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, 1952a,b,c, 1987), Fumi & Ripamonti (1980a,b), Nowick (1995), Nye (1957, 1985), Sands (1995), Sirotnin & 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).