

1.1. INTRODUCTION TO THE PROPERTIES OF TENSORS

(i) The submatrices associated with the principal properties are symmetric with respect to interchange of the indices related to the causes and to the effects: these properties are represented by symmetric tensors. For instance, the dielectric constant and the elastic constants are represented by symmetric tensors of rank 2 and 4, respectively (see Section 1.1.3.4).

(ii) The submatrices associated with terms that are symmetric with respect to the main diagonal of matrices (C) and (R) and that represent cross effects are transpose to one another. For instance, matrix (C_S^E) representing the converse piezoelectric effect is the transpose of matrix (C_P^T) representing the piezoelectric effect. It will be shown in Section 1.1.3.4 that they are the components of tensors of rank 3.

1.1.1.5. Onsager relations

Let us now consider systems that are in steady state and not in thermodynamic equilibrium. The intensive and extensive parameters are time dependent and relation (1.1.1.3) can be written

$$J_m = L_{mn}X_n,$$

where the intensive parameters X_n are, for instance, a temperature gradient, a concentration gradient, a gradient of electric potential. The corresponding extensive parameters J_m are the heat flow, the diffusion of matter and the current density. The diagonal terms of matrix L_{mn} correspond to thermal conductivity (Fourier's law), diffusion coefficients (Fick's law) and electric conductivity (Ohm's law), respectively. Non-diagonal terms correspond to cross effects such as the thermoelectric effect, thermal diffusion etc. All the properties corresponding to these examples are represented by tensors of rank 2. The case of second-rank axial tensors where the symmetrical part of the tensors changes sign on time reversal was discussed by Zheludev (1986).

The Onsager reciprocity relations (Onsager, 1931a,b)

$$L_{mn} = L_{nm}$$

express the symmetry of matrix L_{mn}. They are justified by considerations of statistical thermodynamics and are not as obvious as those expressing the symmetry of matrix (C_P^Q). For instance, the symmetry of the tensor of rank 2 representing thermal conductivity is associated with the fact that a circulating flow is undetectable.

Transport properties are described in Chapter 1.8 of this volume.

1.1.2. Basic properties of vector spaces

[The reader may also refer to Section 1.1.4 of Volume B of International Tables for Crystallography (2000).]

1.1.2.1. Change of basis

Let us consider a vector space spanned by the set of n basis vectors e₁, e₂, e₃, . . . , e_n. The decomposition of a vector using this basis is written

$$\mathbf{x} = x^i \mathbf{e}_i \tag{1.1.2.1}$$

using the Einstein convention. The interpretation of the position of the indices is given below. For the present, we shall use the simple rules:

- (i) the index is a subscript when attached to basis vectors;
- (ii) the index is a superscript when attached to the components. The components are numerical coordinates and are therefore dimensionless numbers.

Let us now consider a second basis, e'_j. The vector x is independent of the choice of basis and it can be decomposed also in the second basis:

$$\mathbf{x} = x'^i \mathbf{e}'_i. \tag{1.1.2.2}$$

If Aⁱ_j and B^j_i are the transformation matrices between the bases e_i and e'_j, the following relations hold between the two bases:

$$\left. \begin{aligned} \mathbf{e}_i &= A^j_i \mathbf{e}'_j; & \mathbf{e}'_j &= B^i_j \mathbf{e}_i \\ x^i &= B^i_j x'^j; & x'^j &= A^j_i x^i \end{aligned} \right\} \tag{1.1.2.3}$$

(summations over j and i, respectively). The matrices Aⁱ_j and B^j_i are inverse matrices:

$$A^i_j B^k_j = \delta^k_i \tag{1.1.2.4}$$

(Kronecker symbol: δ^k_i = 0 if i ≠ k, = 1 if i = k).

Important Remark. The behaviour of the basis vectors and of the components of the vectors in a transformation are different. The roles of the matrices Aⁱ_j and B^j_i are opposite in each case. The components are said to be *contravariant*. Everything that transforms like a basis vector is *covariant* and is characterized by an *inferior* index. Everything that transforms like a component is *contravariant* and is characterized by a *superior* index. The property describing the way a mathematical body transforms under a change of basis is called *variance*.

1.1.2.2. Metric tensor

We shall limit ourselves to a *Euclidean* space for which we have defined the scalar product. The analytical expression of the scalar product of two vectors x = xⁱe_i and y = y^je_j is

$$\mathbf{x} \cdot \mathbf{y} = x^i \mathbf{e}_i \cdot y^j \mathbf{e}_j.$$

Let us put

$$\mathbf{e}_i \cdot \mathbf{e}_j = g_{ij}. \tag{1.1.2.5}$$

The nine components g_{ij} are called the components of the *metric tensor*. Its tensor nature will be shown in Section 1.1.3.6.1. Owing to the commutativity of the scalar product, we have

$$g_{ij} = \mathbf{e}_i \cdot \mathbf{e}_j = \mathbf{e}_j \cdot \mathbf{e}_i = g_{ji}.$$

The table of the components g_{ij} is therefore symmetrical. One of the definition properties of the scalar product is that if x · y = 0 for all x, then y = 0. This is translated as

$$x^i y^j g_{ij} = 0 \quad \forall x^i \implies y^j g_{ij} = 0.$$

In order that only the trivial solution (y^j = 0) exists, it is necessary that the determinant constructed from the g_{ij}'s is different from zero:

$$\Delta(g_{ij}) \neq 0.$$

This important property will be used in Section 1.1.2.4.1.

1.1.2.3. Orthonormal frames of coordinates – rotation matrix

An orthonormal coordinate frame is characterized by the fact that

$$g_{ij} = \delta_{ij} \quad (= 0 \text{ if } i \neq j \text{ and } = 1 \text{ if } i = j). \tag{1.1.2.6}$$

One deduces from this that the scalar product is written simply as

$$\mathbf{x} \cdot \mathbf{y} = x^i y^j g_{ij} = x^i y^i.$$

Let us consider a change of basis between two orthonormal systems of coordinates:

$$\mathbf{e}_i = A^j_i \mathbf{e}'_j.$$

Multiplying the two sides of this relation by e'_j, it follows that