(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, 1931*a*,*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 $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3, \ldots, \mathbf{e}_n$. The decomposition of a vector using this basis is written

$$\mathbf{x} = x^i \mathbf{e}_i \qquad (1.1.2.1)$$

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, $\mathbf{e}'_j$. The vector $\mathbf{x}$ is independent of the choice of basis and it can be decomposed also in the second basis:

$$\mathbf{x} = x'^i \mathbf{e}'_i. \qquad (1.1.2.2)$$

If A_i^j and B_j^i are the transformation matrices between the bases $\mathbf{e}_i$ and $\mathbf{e}'_j$, the following relations hold between the two bases:

$$\left.\begin{array}{ll} \mathbf{e}_i = A_i^j \mathbf{e}'_j; & \mathbf{e}'_j = B_j^i \mathbf{e}_i \\ x^i = B_j^i x'^j; & x'^j = A_i^j x^i \end{array}\right\} \qquad (1.1.2.3)$$

(summations over j and i, respectively). The matrices A_i^j and B_j^i are inverse matrices:

$$A_i^j B_j^k = \delta_i^k \qquad (1.1.2.4)$$

(Kronecker symbol: $\delta_i^k = 0$ if $i \neq k$, $= 1$ 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 A_i^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 $\mathbf{x} = x^i \mathbf{e}_i$ and $\mathbf{y} = y^j \mathbf{e}_j$ is

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

Let us put

$$\mathbf{e}_i \cdot \mathbf{e}_j = g_{ij}. \qquad (1.1.2.5)$$

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 $\mathbf{x} \cdot \mathbf{y} = 0$ for all $\mathbf{x}$, then $\mathbf{y} = \mathbf{0}$. This is translated as

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

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

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

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:

$$\mathbf{e}_i = A_i^j \mathbf{e}'_j.$$

Multiplying the two sides of this relation by $\mathbf{e}'_j$, it follows that