International Tables for Crystallography (2006). Vol. D, Section 1.1.1.4, pp. 4–5.

(iv) *Expansion in Taylor series of a field of vectors*. Let us consider a field of vectors $\mathbf{u}(\mathbf{r})$ where $\mathbf{r}$ is a position vector. The Taylor expansion of its components is given by

$$u^i(\mathbf{r}+\mathrm{d}\mathbf{r}) = u^i(\mathbf{r}) + \left(\frac{\partial u^i}{\partial u^j}\right)\mathrm{d}x^j + \tfrac{1}{2}\left(\frac{\partial^2 u^i}{\partial u^j \partial u^k}\right)\mathrm{d}x^j\ \mathrm{d}x^k + \dots \quad (1.1.1.2)$$

using the so-called Einstein convention, which implies that there is automatically a summation each time the same index appears twice, once as a superscript and once as a subscript. This index is called a *dummy* index. It will be shown in Section 1.1.3.8 that the nine partial differentials $\partial u^i/\partial x^j$ and the 27 partial differentials $\partial^2 u^i/(\partial x^j \partial x^k)$ are the components of tensors of rank 2 and 3, respectively.

Remark. Of the four examples given above, the first three (thermal expansion, dielectric constant, stressed rod) are related to *physical property tensors* (also called *material tensors*), which are characteristic of the medium and whose components have the same value everywhere in the medium if the latter is homogeneous, while the fourth one (expansion in Taylor series of a field of vectors) is related to a *field tensor* whose components vary at every point of the medium. This is the case, for instance, for the strain and for the stress tensors (see Sections 1.3.1 and 1.3.2).

1.1.1.3. *The matrix of physical properties*

Each extensive parameter is in principle a function of all the intensive parameters. For a variation $\mathrm{d}i_q$ of a particular intensive parameter, there will be a variation $\mathrm{d}e_p$ of every extensive parameter. One may therefore write

$$\mathrm{d}e_p = C_p^q\ \mathrm{d}i_q. \quad (1.1.1.3)$$

The summation is over all the intensive parameters that have varied.

One may use a matrix notation to write the equations relating the variations of each extensive parameter to the variations of all the intensive parameters:

$$(\mathrm{d}e) = (C)(\mathrm{d}i), \quad (1.1.1.4)$$

where the intensive and extensive parameters are arranged in column matrices, $(\mathrm{d}i)$ and $(\mathrm{d}e)$, respectively. In a similar way, one could write the relations between intensive and extensive parameters as

$$\left.\begin{aligned} \mathrm{d}i_p &= R_p^q\ \mathrm{d}e_q \\ (\mathrm{d}i) &= (R)(\mathrm{d}e). \end{aligned}\right\} \quad (1.1.1.5)$$

Matrices (C) and (R) are inverse matrices. Their leading diagonal terms relate an extensive parameter and the associated intensive parameter (their product has the dimensions of energy), *e.g.* the elastic constants, the dielectric constant, the specific heat *etc.* The corresponding physical properties are called principal properties. If one only of the intensive parameters, i_q, varies, a variation $\mathrm{d}i_q$ of this parameter is the *cause* of which the *effect* is a variation,

$$\mathrm{d}e_p = C_p^q\ \mathrm{d}i_q$$

(*without summation*), of each of the extensive parameters. The matrix coefficients C_p^q may therefore be considered as partial differentials:

$$C_p^q = \partial e_p/\partial i_q.$$

The parameters C_p^q that relate causes $\mathrm{d}i_q$ and effects $\mathrm{d}e_p$ represent physical properties and matrix (C) is called the *matrix of physical properties*. Let us consider the following intensive parameters: T stress, $\mathbf{E}$ electric field, $\mathbf{H}$ magnetic field, Θ temperature and the associated extensive parameters: S strain, $\mathbf{P}$ electric polarization, $\mathbf{B}$ magnetic induction, σ entropy, respectively. Matrix equation (1.1.1.4) may then be written:

$$\begin{pmatrix} S \\ P \\ B \\ \delta\sigma \end{pmatrix} = \begin{pmatrix} C_S^T & C_S^E & C_S^H & C_S^\Theta \\ C_P^T & C_P^E & C_P^H & C_P^\Theta \\ C_B^T & C_B^E & C_B^H & C_B^\Theta \\ C_\sigma^T & C_\sigma^E & C_\sigma^H & C_\sigma^\Theta \end{pmatrix} \begin{pmatrix} T \\ E \\ H \\ \Theta \end{pmatrix}. \quad (1.1.1.6)$$

The various intensive and extensive parameters are represented by scalars, vectors or tensors of higher rank, and each has several components. The terms of matrix (C) are therefore actually submatrices containing all the coefficients C_p^q relating all the components of a given extensive parameter to the components of an intensive parameter. The leading diagonal terms, C_S^T, C_P^E, C_B^H, C_σ^Θ, correspond to the principal physical properties, which are elasticity, dielectric susceptibility, magnetic susceptibility and specific heat, respectively. The non-diagonal terms are also associated with physical properties, but they relate intensive and extensive parameters whose products do not have the dimension of energy. They may be coupled in pairs symmetrically with respect to the main diagonal:

C_S^E and C_P^T represent the piezoelectric effect and the converse piezoelectric effect, respectively;

C_S^H and C_B^T the piezomagnetic effect and the converse piezomagnetic effect;

C_S^Θ and C_σ^T thermal expansion and the piezocalorific effect;

C_P^T and C_σ^E the pyroelectric and the electrocalorific effects;

C_P^H and C_B^E the magnetoelectric effect and the converse magnetoelectric effect;

C_σ^H and C_B^Θ the pyromagnetic effect and the magnetocalorific effect.

It is important to note that equation (1.1.1.6) is of a thermodynamic nature and simply provides a general framework. It indicates the possibility for a given physical property to exist, but in no way states that a given material will exhibit it. Curie laws, which will be described in Section 1.1.4.2, show for instance that certain properties such as pyroelectricity or piezoelectricity may only appear in crystals that belong to certain point groups.

1.1.1.4. *Symmetry of the matrix of physical properties*

If parameter e_p varies by $\mathrm{d}e_p$, the specific energy varies by $\mathrm{d}u$, which is equal to

$$\mathrm{d}u = i_p\ \mathrm{d}e_p.$$

We have, therefore

$$i_p = \frac{\partial u}{\partial e_p}$$

and, using (1.1.1.5),

$$R_p^q = \frac{\partial i_p}{\partial e_q} = \frac{\partial^2 u}{\partial e_p \partial e_q}.$$

Since the energy is a state variable with a perfect differential, one can interchange the order of the differentiations:

$$R_p^q = \frac{\partial^2 u}{\partial e_q \partial e_p} = \frac{\partial i_q}{\partial e_p}.$$

Since p and q are dummy indices, they may be exchanged and the last term of this equation is equal to R_q^p. It follows that

$$R_p^q = R_q^p.$$

Matrices R_p^q and C_p^q are therefore symmetric. We may draw two important conclusions from this result:

(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

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

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

references