International Tables for Crystallography (2006). Vol. D, Section 1.1.2.3, pp. 5–6.

(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:

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

(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

$$\mathbf{e}_i \cdot \mathbf{e}'_j = A_i^j \mathbf{e}'_k \cdot e'_j = A_i^j g'_{kj} = A_i^j \delta_{kj} \quad \text{(written correctly)},$$

which can also be written, if one notes that variance is not apparent in an orthonormal frame of coordinates and that the position of indices is therefore not important, as

$$\mathbf{e}_i \cdot \mathbf{e}'_j = A_i^j \quad \text{(written incorrectly)}.$$

The matrix coefficients, A_i^j, are the direction cosines of $\mathbf{e}'_j$ with respect to the $\mathbf{e}_i$ basis vectors. Similarly, we have

$$B_j^i = \mathbf{e}_i \cdot \mathbf{e}'_j$$

so that

$$A_i^j = B_j^i \quad \text{or} \quad A = B^T,$$

where ^{T} indicates transpose. It follows that

$$A = B^T \text{ and } A = B^{-1}$$

so that

$$\left.\begin{array}{lll} A^T = A^{-1} & \Rightarrow & A^T A = I \\ B^T = B^{-1} & \Rightarrow & B^T B = I. \end{array}\right\} \qquad (1.1.2.7)$$

The matrices A and B are unitary matrices or matrices of rotation and

$$\Delta(A)^2 = \Delta(B)^2 = 1 \Rightarrow \Delta(A) = \pm 1. \qquad (1.1.2.8)$$

If $\Delta(A) = 1$ the senses of the axes are not changed – *proper* rotation.

If $\Delta(A) = -1$ the senses of the axes are changed – *improper* rotation. (The right hand is transformed into a left hand.)

One can write for the coefficients A_i^j

$$A_i^j B_j^k = \delta_i^k; \quad A_i^j A_j^k = \delta_i^k,$$

giving six relations between the nine coefficients A_i^j. There are thus *three* independent coefficients of the 3×3 matrix A.

1.1.2.4. *Covariant coordinates – dual or reciprocal space*

1.1.2.4.1. *Covariant coordinates*

Using the developments (1.1.2.1) and (1.1.2.5), the scalar products of a vector $\mathbf{x}$ and of the basis vectors $\mathbf{e}_i$ can be written

$$x_i = \mathbf{x} \cdot \mathbf{e}_i = x^j \mathbf{e}_j \cdot \mathbf{e}_i = x^j g_{ij}. \qquad (1.1.2.9)$$

The n quantities x_i are called *covariant* components, and we shall see the reason for this a little later. The relations (1.1.2.9) can be considered as a system of equations of which the components x^j are the unknowns. One can solve it since $\Delta(g_{ij}) \neq 0$ (see the end of Section 1.1.2.2). It follows that

$$x^j = x_i g^{ij} \qquad (1.1.2.10)$$

with

$$g^{ij} g_{jk} = \delta_k^i. \qquad (1.1.2.11)$$

The table of the g^{ij}'s is the inverse of the table of the g_{ij}'s. Let us now take up the development of $\mathbf{x}$ with respect to the basis $\mathbf{e}_i$:

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

Let us replace x^i by the expression (1.1.2.10):

$$\mathbf{x} = x_j g^{ij} \mathbf{e}_i, \qquad (1.1.2.12)$$

and let us introduce the set of n vectors

$$\mathbf{e}^j = g^{ij} \mathbf{e}_i \qquad (1.1.2.13)$$

which span the space E^n $(j = 1, \ldots, n)$. *This set of n vectors forms a basis* since (1.1.2.12) can be written with the aid of (1.1.2.13) as

$$\mathbf{x} = x_j \mathbf{e}^j. \qquad (1.1.2.14)$$

The x_j's are the components of $\mathbf{x}$ in the basis $\mathbf{e}^j$. This basis is called the *dual basis*. By using (1.1.2.11) and (1.1.2.13), one can show in the same way that

$$\mathbf{e}_j = g_{ij} \mathbf{e}^j. \qquad (1.1.2.15)$$

It can be shown that the basis vectors $\mathbf{e}^j$ transform in a change of basis like the components x^j of the physical space. They are therefore *contravariant*. In a similar way, the components x_j of a vector $\mathbf{x}$ with respect to the basis $\mathbf{e}^j$ transform in a change of basis like the basis vectors in direct space, $\mathbf{e}_j$; they are therefore *covariant*:

$$\left.\begin{array}{ll} \mathbf{e}^j = B_k^j \mathbf{e}'^k; & \mathbf{e}'^k = A_j^k \mathbf{e}^j \\ x_i = A_i^j x'_j; & x'_j = B_j^i x_i. \end{array}\right\} \qquad (1.1.2.16)$$

1.1.2.4.2. *Reciprocal space*

Let us take the scalar products of a covariant vector $\mathbf{e}_i$ and a contravariant vector $\mathbf{e}^j$:

$$\mathbf{e}_i \cdot \mathbf{e}^j = \mathbf{e}_i \cdot g^{jk} \mathbf{e}_k = \mathbf{e}_i \cdot \mathbf{e}_k g^{jk} = g_{ik} g^{jk} = \delta_i^j$$

[using expressions (1.1.2.5), (1.1.2.11) and (1.1.2.13)].

The relation we obtain, $\mathbf{e}_i \cdot \mathbf{e}^j = \delta_i^j$, is identical to the relations defining the reciprocal lattice in crystallography; *the reciprocal basis then is identical to the dual basis* $\mathbf{e}^i$.

1.1.2.4.3. *Properties of the metric tensor*

In a change of basis, following (1.1.2.3) and (1.1.2.5), the g_{ij}'s transform according to

$$\left.\begin{array}{l} g_{ij} = A_i^k A_j^m g'_{km} \\ g'_{ij} = B_i^k B_j^m g_{km}. \end{array}\right\} \qquad (1.1.2.17)$$

Let us now consider the scalar products, $\mathbf{e}^i \cdot \mathbf{e}^j$, of two contravariant basis vectors. Using (1.1.2.11) and (1.1.2.13), it can be shown that

$$\mathbf{e}^i \cdot \mathbf{e}^j = g^{ij}. \qquad (1.1.2.18)$$

In a change of basis, following (1.1.2.16), the g^{ij}'s transform according to

$$\left.\begin{array}{l} g^{ij} = B_k^i B_m^j g'^{km} \\ g'^{ij} = A_k^i A_m^j g^{km}. \end{array}\right\} \qquad (1.1.2.19)$$

The volumes V' and V of the cells built on the basis vectors $\mathbf{e}'_i$ and $\mathbf{e}_i$, respectively, are given by the triple scalar products of these two sets of basis vectors and are related by

$$\begin{aligned} V' &= (\mathbf{e}'_1, \mathbf{e}'_2, \mathbf{e}'_3) \\ &= \Delta(B_j^i)(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3) \\ &= \Delta(B_j^i) V, \end{aligned} \qquad (1.1.2.20)$$

where $\Delta(B_j^i)$ is the determinant associated with the transformation matrix between the two bases. From (1.1.2.17) and (1.1.2.20), we can write

$$\Delta(g'_{ij}) = \Delta(B_i^k)\Delta(B_j^m)\Delta(g_{km}).$$

references