1.1. Introduction to the properties of tensors

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1.1.1. The matrix of physical properties

1.1.1.1. *Notion of extensive and intensive quantities*

Physical laws express in general the response of a medium to a certain influence. Most physical properties may therefore be defined by a relation coupling two or more measurable quantities. For instance, the specific heat characterizes the relation between a variation of temperature and a variation of entropy at a given temperature in a given medium, the dielectric susceptibility the relation between electric field and electric polarization, the elastic constants the relation between an applied stress and the resulting strain *etc*. These relations are between quantities of the same nature: thermal, electrical and mechanical, respectively. But there are also cross effects, for instance:

(*a*) *thermal expansion* and *piezocalorific effect*: mechanical reaction to a thermal impetus or the reverse;

(*b*) *pyroelectricity* and *electrocalorific effect*: electrical response to a thermal impetus or the reverse;

(*c*) *piezoelectricity* and *electrostriction*: electric response to a mechanical impetus;

(*d*) *piezomagnetism* and *magnetostriction*: magnetic response to a mechanical impetus;

(*e*) *photoelasticity*: birefringence produced by stress;

(*f*) *acousto-optic effect*: birefringence produced by an acoustic wave;

(*g*) *electro-optic effect*: birefringence produced by an electric field;

(*h*) *magneto-optic effect*: appearance of a rotatory polarization under the influence of a magnetic field.

The physical quantities that are involved in these relations can be divided into two categories:

(i) *extensive quantities*, which are proportional to the volume of matter or to the mass, that is to the number of molecules in the medium, for instance entropy, energy, quantity of electricity *etc*. One uses frequently specific extensive parameters, which are given per unit mass or per unit volume, such as the specific mass, the electric polarization (dipole moment per unit volume) *etc*.

(ii) *intensive parameters*, quantities whose product with an extensive quantity is homogeneous to an energy. For instance, volume is an extensive quantity; the energy stored by a gas undergoing a change of volume dV under pressure p is p dV. Pressure is therefore the intensive parameter associated with volume. Table 1.1.1.1 gives examples of extensive quantities and of the related intensive parameters.

1.1.1.2. *Notion of tensor in physics*

Each of the quantities mentioned in the preceding section is represented by a mathematical expression. Some are direction independent and are represented by *scalars*: specific mass, specific heat, volume, pressure, entropy, temperature, quantity of electricity, electric potential. Others are direction dependent and are represented by *vectors*: force, electric field, electric displacement, the gradient of a scalar quantity. Still others cannot be represented by scalars or vectors and are represented by more complicated mathematical expressions. Magnetic quantities are represented by *axial* vectors (or pseudovectors), which are a particular kind of tensor (see Section 1.1.4.5.3). A few examples will show the necessity of using tensors in physics and Section 1.1.3 will present elementary mathematical properties of tensors.

(i) *Thermal expansion*. In an isotropic medium, thermal expansion is represented by a single number, a scalar, but this is not the case in an anisotropic medium: a sphere cut in an anisotropic medium becomes an ellipsoid when the temperature is varied and thermal expansion can no longer be represented by a single number. It is actually represented by a tensor of rank 2.

(ii) *Dielectric constant*. In an isotropic medium of a perfect dielectric we can write, in SI units,

$$\mathbf{P} = \varepsilon_0 \chi_e \mathbf{E}$$
$$\mathbf{D} = \varepsilon_0 \mathbf{E} + \mathbf{P} = \varepsilon_0 (1 + \chi_e)\mathbf{E} = \varepsilon\mathbf{E},$$

where $\mathbf{P}$ is the electric polarization (= dipole moment per unit volume), ε_0 the permittivity of vacuum, χ_e the dielectric susceptibility, $\mathbf{D}$ the electric displacement and ε the dielectric constant, also called dielectric permittivity. These expressions indicate that the electric field, on the one hand, and polarization and displacement, on the other hand, are linearly related. In the general case of an anisotropic medium, this is no longer true and one must write expressions indicating that the components of the displacement are linearly related to the components of the field:

$$\begin{cases} D^1 = \varepsilon_1^1 E^1 + \varepsilon_1^2 E^2 + \varepsilon_1^3 E \\ D^2 = \varepsilon_1^2 E^1 + \varepsilon_2^2 E^2 + \varepsilon_2^3 E \\ D^3 = \varepsilon_1^3 E^1 + \varepsilon_2^3 E^2 + \varepsilon_3^3 E. \end{cases} \qquad (1.1.1.1)$$

The dielectric constant is now characterized by a set of nine components ε_i^j; they are the components of a tensor of rank 2. It will be seen in Section 1.1.4.5.2.1 that this tensor is symmetric ($\varepsilon_i^j = \varepsilon_j^i$) and that the number of independent components is equal to six.

(iii) *Stressed rod (Hooke's law)*. If one pulls a rod of length ℓ and cross section $\mathcal{A}$ with a force F, its length is increased by a quantity $\Delta\ell$ given by $\Delta\ell/\ell = (1/E)F/\mathcal{A}$, where E is Young's modulus, or elastic stiffness (see Section 1.3.3.1). But, at the same time, the radius, r, decreases by Δr given by $\Delta r/r = -(\nu/E)F/\mathcal{A}$, where ν is Poisson's ratio (Section 1.3.3.4.3). It can be seen that a scalar is not sufficient to describe the elastic deformation of a material, even if it is isotropic. The number of independent components depends on the symmetry of the medium and it will be seen that they are the components of a tensor of rank 4. It was precisely to describe the properties of elasticity by a mathematical expression that the notion of a tensor was introduced in physics by W. Voigt in the 19th century (Voigt, 1910) and by L. Brillouin in the first half of the 20th century (Brillouin, 1949).

Table 1.1.1.1. *Extensive quantities and associated intensive parameters*

The last four lines of the table refer to properties that are time dependent.

Extensive quantities	Intensive parameters
Volume	Pressure
Strain	Stress
Displacement	Force
Entropy	Temperature
Quantity of electricity	Electric potential
Electric polarization	Electric field
Electric displacement	Electric field
Magnetization	Magnetic field
Magnetic induction	Magnetic field
Reaction rate	Chemical potential
Heat flow	Temperature gradient
Diffusion of matter	Concentration gradient
Electric current	Potential gradient

(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

$$u^i(\mathbf{r} + d\mathbf{r}) = u^i(\mathbf{r}) + \left(\frac{\partial u^i}{\partial u^j}\right) dx^j + \tfrac{1}{2}\left(\frac{\partial^2 u^i}{\partial u^j \partial u^k}\right) dx^j \ dx^k + \ldots$$

$$(1.1.1.2)$$

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 di_q of a particular intensive parameter, there will be a variation de_p of every extensive parameter. One may therefore write

$$de_p = C_p^q \ di_q. \qquad (1.1.1.3)$$

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:

$$(de) = (C)(di), \qquad (1.1.1.4)$$

where the intensive and extensive parameters are arranged in column matrices, (di) and (de), respectively. In a similar way, one could write the relations between intensive and extensive parameters as

$$\left.\begin{array}{ll} di_p & = R_p^q \ de_q \\ (di) & = (R)(de). \end{array}\right\} \qquad (1.1.1.5)$$

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 di_q of this parameter is the *cause* of which the *effect* is a variation,

$$de_p = C_p^q \ di_q$$

(*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 di_q and effects de_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:

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

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 de_p, the specific energy varies by du, which is equal to

$$du = i_p \ de_p.$$

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

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

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

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

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:

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

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

$$A_i^j B_j^k = \delta_i^k \tag{1.1.2.4}$$

(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

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

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

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

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

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

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:

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

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

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

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

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

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

$$B^i_j = \mathbf{e}_i \cdot \mathbf{e}'_j$$

so that

$$A^j_i = B^i_j \quad \text{or} \quad A = B^T,$$

where ^{T} indicates transpose. It follows that

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

so that

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

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^j_i

$$A^j_i B^k_j = \delta^k_i; \quad A^j_i A^k_j = \delta^k_i,$$

giving six relations between the nine coefficients A^j_i. 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

$$g^{ij} g_{jk} = \delta^i_k. \qquad (1.1.2.11)$$

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*:

$$\left.\begin{array}{ll} \mathbf{e}^j = B^j_k \mathbf{e}'^k; & \mathbf{e}'^k = A^k_j \mathbf{e}^j \\ x_i = A^j_i x'_j; & x'_j = B^i_j x_i. \end{array}\right\} \qquad (1.1.2.16)$$

1.1.2.4.2. *Reciprocal space*

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

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

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

The relation we obtain, $\mathbf{e}_i \cdot \mathbf{e}^j = \delta^j_i$, 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

$$\left.\begin{array}{l} g_{ij} = A^k_i A^m_j g'_{km} \\ g'_{ij} = B^k_i B^m_j g_{km}. \end{array}\right\} \qquad (1.1.2.17)$$

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

$$\left.\begin{array}{l} g^{ij} = B^i_k B^j_m g'^{km} \\ g'^{ij} = A^i_k A^j_m g^{km}. \end{array}\right\} \qquad (1.1.2.19)$$

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

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

where $\Delta(B^i_j)$ 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

$$\Delta(g'_{ij}) = \Delta(B^k_i) \Delta(B^m_j) \Delta(g_{km}).$$

If the basis $\mathbf{e}_i$ is orthonormal, $\Delta(g_{km})$ and V are equal to one, $\Delta(B_j)$ is equal to the volume V' of the cell built on the basis vectors $\mathbf{e}'_i$ and

$$\Delta(g'_{ij}) = V'^2.$$

This relation is actually general and one can remove the prime index:

$$\Delta(g_{ij}) = V^2. \tag{1.1.2.21}$$

In the same way, we have for the corresponding reciprocal basis

$$\Delta(g^{ij}) = V^{*2},$$

where V^* is the volume of the reciprocal cell. Since the tables of the g_{ij}'s and of the g^{ij}'s are inverse, so are their determinants, and therefore the volumes of the unit cells of the direct and reciprocal spaces are also inverse, which is a very well known result in crystallography.

1.1.3. Mathematical notion of tensor

1.1.3.1. *Definition of a tensor*

For the mathematical definition of tensors, the reader may consult, for instance, Lichnerowicz (1947), Schwartz (1975) or Sands (1995).

1.1.3.1.1. *Linear forms*

A linear form in the space E_n is written

$$T(\mathbf{x}) = t_i x^i,$$

where $T(\mathbf{x})$ is independent of the chosen basis and the t_i's are the coordinates of T in the dual basis. Let us consider now a *bilinear* form in the product space $E_n \otimes F_p$ of two vector spaces with n and p dimensions, respectively:

$$T(\mathbf{x}, \mathbf{y}) = t_{ij} x^i y^j.$$

The np quantities t_{ij}'s are, *by definition*, the components of a tensor of rank 2 and the form $T(\mathbf{x}, \mathbf{y})$ is *invariant* if one changes the basis in the space $E_n \otimes F_p$. The tensor t_{ij} is said to be *twice covariant*. It is also possible to construct a bilinear form by replacing the spaces E_n and F_p by their respective conjugates E^n and F^p. Thus, one writes

$$T(\mathbf{x}, \mathbf{y}) = t_{ij} x^i y^j = t^j_i x^i y_j = t^i_j x_i y^j = t^{ij} x_i y_j,$$

where t^{ij} is the doubly contravariant form of the tensor, whereas t^j_i and t^i_j are mixed, once covariant and once contravariant.

We can generalize by defining in the same way tensors of rank 3 or higher by using trilinear or multilinear forms. A vector is a tensor of rank 1, and a scalar is a tensor of rank 0.

1.1.3.1.2. *Tensor product*

Let us consider two vector spaces, E_n with n dimensions and F_p with p dimensions, and let there be two linear forms, $T(\mathbf{x})$ in E_n and $S(\mathbf{y})$ in F_p. We shall associate with these forms a bilinear form called a *tensor product* which belongs to the product space with np dimensions, $E_n \otimes F_p$:

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

This correspondence possesses the following properties:
(i) it is distributive from the right and from the left;
(ii) it is associative for multiplication by a scalar;
(iii) the tensor products of the vectors with a basis E_n and those with a basis F_p constitute a basis of the product space.
The analytical expression of the tensor product is then

$$\left.\begin{array}{l} T(\mathbf{x}) = t_i x^j \\ S(\mathbf{y}) = s_j y^i \end{array}\right\} P(\mathbf{x}, \mathbf{y}) = p_{ij} x^i y^j = t_i x^i s_j y^j = t_i s_j x^i y^j.$$

One deduces from this that

$$p_{ij} = t_i s_j.$$

It is a tensor of rank 2. One can equally well envisage the tensor product of more than two spaces, for example, $E_n \otimes F_p \otimes G_q$ in npq dimensions. We shall limit ourselves in this study to the case of *affine* tensors, which are defined in a space constructed from the product of the space E_n with itself or with its conjugate E^n. Thus, a tensor product of rank 3 will have n^3 components. The tensor product can be generalized as the product of multilinear forms. One can write, for example,

$$\left.\begin{array}{l} P(\mathbf{x}, \mathbf{y}, \mathbf{z}) = T(\mathbf{x}, \mathbf{y}) \otimes S(\mathbf{z}) \\ p^j_{ik} x^i y_j z^k = t^j_i x^i y_j s_k z^k. \end{array}\right\} \tag{1.1.3.1}$$

1.1.3.2. *Behaviour under a change of basis*

A multilinear form is, by definition, invariant under a change of basis. Let us consider, for example, the trilinear form (1.1.3.1). If we change the system of coordinates, the components of vectors $\mathbf{x}$, $\mathbf{y}$, $\mathbf{z}$ become

$$x^i = B^i_\alpha x'^\alpha; \quad y_j = A^\beta_j y'_\beta; \quad z^k = B^k_\gamma z'^\gamma.$$

Let us put these expressions into the trilinear form (1.1.3.1):

$$P(\mathbf{x}, \mathbf{y}, \mathbf{z}) = p^j_{ik} B^i_\alpha x'^\alpha A^\beta_j y'_\beta B^k_\gamma z'^\gamma.$$

Now we can equally well make the components of the tensor appear in the new basis:

$$P(\mathbf{x}, \mathbf{y}, \mathbf{z}) = p'^\beta_{\alpha\gamma} x'^\alpha y'_\beta z'^\gamma.$$

As the decomposition is unique, one obtains

$$p'^\beta_{\alpha\gamma} = p^j_{ik} B^i_\alpha A^\beta_j B^k_\gamma. \tag{1.1.3.2}$$

One thus deduces the rule for transforming the components of a tensor q times covariant and r times contravariant: they transform like the product of q covariant components and r contravariant components.

This transformation rule can be taken inversely as the definition of the components of a tensor of rank $n = q + r$.

Example. The operator O representing a symmetry operation has the character of a tensor. In fact, under a change of basis, O transforms into O':

$$O' = AOA^{-1}$$

so that

$$O'^i_j = A^i_k O^k_l (A^{-1})^l_j.$$

Now the matrices A and B are inverses of one another:

$$O'^i_j = A^i_k O^k_l B^l_j.$$

The symmetry operator is a tensor of rank 2, once covariant and once contravariant.

1.1.3.3. *Operations on tensors*

1.1.3.3.1. *Addition*

It is necessary that the tensors are of the same nature (same rank and same variance).

1.1.3.3.2. *Multiplication by a scalar*

This is a particular case of the tensor product.

1.1.3.3.3. *Contracted product, contraction*

Here we are concerned with an operation that only exists in the case of tensors and that is very important because of its applications in physics. In practice, it is almost always the case that tensors enter into physics through the intermediary of a contracted product.

(i) *Contraction*. Let us consider a tensor of rank 2 that is once covariant and once contravariant. Let us write its transformation in a change of coordinate system:

$$t_i^{\prime j} = A_p^j B_i^q t_q^p.$$

Now consider the quantity $t_i^{\prime i}$ derived by applying the Einstein convention ($t_i^{\prime i} = t_1^{\prime 1} + t_2^{\prime 2} + t_3^{\prime 3}$). It follows that

$$t_i^{\prime i} = A_p^i B_i^q t_q^p = \delta_p^q t_q^q$$
$$t_i^{\prime i} = t_p^p.$$

This is an invariant quantity and so is a *scalar*. This operation can be carried out on any tensor of rank higher than or equal to two, provided that it is expressed in a form such that its components are (at least) once covariant and once contravariant.

The *contraction* consists therefore of equalizing a covariant index and a contravariant index, and then in summing over this index. Let us take, for example, the tensor $t_i^{\prime jk}$. Its contracted form is $t_i^{\prime ik}$, which, with a change of basis, becomes

$$t_i^{\prime ik} = A_p^k t_q^{qp}.$$

The components t_i^{ik} are those of a vector, resulting from the contraction of the tensor t_i^{jk}. The rank of the tensor has changed from 3 to 1. In a general manner, the contraction reduces the rank of the tensor from n to $n - 2$.

Example. Let us take again the operator of symmetry O. The trace of the associated matrix is equal to

$$O_1^1 + O_2^2 + O_3^3 = O_i^i.$$

It is the resultant of the contraction of the tensor O. It is a tensor of rank 0, which is a scalar and is invariant under a change of basis.

(ii) *Contracted product*. Consider the product of two tensors of which one is contravariant at least once and the other covariant at least once:

$$p_i^{jk} = t_i^j z^k.$$

If we contract the indices i and k, it follows that

$$p_i^{ji} = t_i^j z^i.$$

The contracted product is then a tensor of rank 1 and not 3. It is an operation that is very frequent in practice.

(iii) *Scalar product*. Next consider the tensor product of two vectors:

$$t_i^j = x_i y^j.$$

After contraction, we get the scalar product:

$$t_i^i = x_i y^i.$$

1.1.3.4. *Tensor nature of physical quantities*

Let us first consider the dielectric constant. In the introduction, we remarked that for an isotropic medium

$$\mathbf{D} = \varepsilon \mathbf{E}.$$

If the medium is anisotropic, we have, for one of the components,

$$D^1 = \varepsilon_1^1 E^1 + \varepsilon_2^1 E^2 + \varepsilon_3^1 E^3.$$

This relation and the equivalent ones for the other components can also be written

$$D^i = \varepsilon_j^i E^j \tag{1.1.3.3}$$

using the Einstein convention.

The scalar product of $\mathbf{D}$ by an arbitrary vector $\mathbf{x}$ is

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

The right-hand member of this relation is a bilinear form that is invariant under a change of basis. The set of nine quantities ε_j^i constitutes therefore the set of components of a tensor of rank 2. Expression (1.1.3.3) is the contracted product of ε_j^i by E^j.

A similar demonstration may be used to show the tensor nature of the various physical properties described in Section 1.1.1, whatever the rank of the tensor. Let us for instance consider the piezoelectric effect (see Section 1.1.4.4.3). The components of the electric polarization, P^i, which appear in a medium submitted to a stress represented by the second-rank tensor T_{jk} are

$$P^i = d^{ijk} T_{jk},$$

where the tensor nature of T_{jk} will be shown in Section 1.3.2. If we take the contracted product of both sides of this equation by any vector of covariant components x_i, we obtain a linear form on the left-hand side, and a trilinear form on the right-hand side, which shows that the coefficients d^{ijk} are the components of a third-rank tensor. Let us now consider the piezo-optic (or photoelastic) effect (see Sections 1.1.4.10.5 and 1.6.7). The components of the variation $\Delta \eta^{ij}$ of the dielectric impermeability due to an applied stress are

$$\Delta \eta^{ij} = \pi^{ijkl} T_{jl}.$$

In a similar fashion, consider the contracted product of both sides of this relation by two vectors of covariant components x_i and y_j, respectively. We obtain a bilinear form on the left-hand side, and a quadrilinear form on the right-hand side, showing that the coefficients π^{ijkl} are the components of a fourth-rank tensor.

1.1.3.5. *Representation surface of a tensor*

1.1.3.5.1. *Definition*

Let us consider a tensor $t_{ijkl...}$ represented in an orthonormal frame where variance is not important. The value of component $t_{1111...}^{\prime}$ in an arbitrary direction is given by

$$t_{1111...}^{\prime} = t_{ijkl...} B_1^i B_1^j B_1^k B_1^l \ldots,$$

where the B_1^i, B_1^j, $\ldots$ are the direction cosines of that direction with respect to the axes of the orthonormal frame.

The *representation surface* of the tensor is the polar plot of $t_{1111...}^{\prime}$.

1.1.3.5.2. *Representation surfaces of second-rank tensors*

The representation surfaces of second-rank tensors are quadrics. The directions of their principal axes are obtained as follows. Let t_{ij} be a second-rank tensor and let $\mathbf{OM} = \mathbf{r}$ be a vector with coordinates x_i. The doubly contracted product, $t_{ij} x^i x^j$, is a scalar. The locus of points M such that

$$t_{ij}x^i x^j = 1$$

is a quadric. Its principal axes are along the directions of the eigenvectors of the matrix with elements t_{ij}. They are solutions of the set of equations

$$t_{ij}x^i = \lambda x^j,$$

where the associated quantities λ are the eigenvalues.

Let us take as axes the principal axes. The equation of the quadric reduces to

$$t_{11}(x^1)^2 + t_{22}(x^2)^2 + t_{33}(x^3)^2 = 1.$$

If the eigenvalues are all of the same sign, the quadric is an ellipsoid; if two are positive and one is negative, the quadric is a hyperboloid with one sheet; if one is positive and two are negative, the quadric is a hyperboloid with two sheets (see Section 1.3.1).

Associated quadrics are very useful for the geometric representation of physical properties characterized by a tensor of rank 2, as shown by the following examples:

(i) *Index of refraction* of a medium. It is related to the dielectric constant by $n = \varepsilon^{1/2}$ and, like it, it is a tensor of rank 2. Its associated quadric is an ellipsoid, the optical indicatrix, which represents its variations with the direction in space (see Section 1.6.3.2).

(ii) *Thermal expansion*. If one cuts a sphere in a medium whose thermal expansion is anisotropic, and if one changes the temperature, the sphere becomes an ellipsoid. Thermal expansion is therefore represented by a tensor of rank 2 (see Chapter 1.4).

(iii) *Thermal conductivity*. Let us place a drop of wax on a plate of gypsum, and then apply a hot point at the centre. There appears a halo where the wax has melted: it is elliptical, indicating anisotropic conduction. Thermal conductivity is represented by a tensor of rank 2 and the elliptical halo of molten wax corresponds to the intersection of the associated ellipsoid with the plane of the plate of gypsum.

1.1.3.5.3. *Representation surfaces of higher-rank tensors*

Examples of representation surfaces of higher-rank tensors are given in Sections 1.3.3.4.4 and 1.9.4.2.

1.1.3.6. *Change of variance of the components of a tensor*

1.1.3.6.1. *Tensor nature of the metric tensor*

Equation (1.1.2.17) describing the behaviour of the quantities $g_{ij} = \mathbf{e}_i \cdot \mathbf{e}_j$ under a change of basis shows that they are the components of a tensor of rank 2, the *metric tensor*. In the same way, equation (1.1.2.19) shows that the g^{ij}'s transform under a change of basis like the product of two contravariant coordinates. The coefficients g^{ij} and g_{ij} are the components of a *unique tensor*, in one case doubly contravariant, in the other case doubly covariant. In a general way, the Euclidean tensors (constructed in a space where one has defined the scalar product) are geometrical entities that can have covariant, contravariant or mixed components.

1.1.3.6.2. *How to change the variance of the components of a tensor*

Let us take a tensor product

$$t^{ij} = x^i y^j.$$

We know that

$$x^i = g^{ik}x_k \quad \text{and} \quad y^j = g^{jl}y_l.$$

It follows that

$$t^{ij} = g^{ik}g^{jl}x_k y_l.$$

$x_k y_l$ is a tensor product of two vectors expressed in the dual space:

$$x_k y_l = t_{kl}.$$

One can thus pass from the doubly covariant form to the doubly contravariant form of the tensor by means of the relation

$$t^{ij} = g^{ik}g^{jl}t_{kl}.$$

This result is general: to change the variance of a tensor (in practice, to raise or lower an index), it is necessary to make the contracted product of this tensor using g^{ij} or g_{ij}, according to the case. For instance,

$$t_k^l = g^{jl}t_{lk}; \quad t_k^{ij} = g_{kl}t^{ijl}.$$

Remark

$$g_j^i = g^{ik}g_{kj} = \delta_j^i.$$

This is a property of the metric tensor.

1.1.3.6.3. *Examples of the use in physics of different representations of the same quantity*

Let us consider, for example, the force, **F**, which is a tensor quantity (tensor of rank 1). One can define it:

(i) by the fundamental law of dynamics:

$$\mathbf{F} = m\mathbf{\Gamma}, \quad \text{with } F^i = m \, \mathrm{d}^2 x^i / \mathrm{d}t^2,$$

where m is the mass and $\mathbf{\Gamma}$ is the acceleration. The force appears here in a *contravariant* form.

(ii) as the derivative of the energy, W:

$$F_i = \partial W / \partial x^i = \partial_i W.$$

The force appears here in *covariant* form. In effect, we shall see in Section 1.1.3.8.1 that to form a derivative with respect to a variable contravariant augments the covariance by unity. The general expression of the law of dynamics is therefore written with the energy as follows:

$$m \, \mathrm{d}^2 x^i / \mathrm{d}t^2 = g^{ij}\partial_j W.$$

1.1.3.7. *Outer product*

1.1.3.7.1. *Definition*

The tensor defined by

$$\mathbf{x} \bigwedge \mathbf{y} = \mathbf{x} \otimes \mathbf{y} - \mathbf{y} \otimes \mathbf{x}$$

is called the *outer product* of vectors **x** and **y**. (*Note*: The symbol is different from the symbol $\wedge$ for the vector product.) The analytical expression of this tensor of rank 2 is

$$\left. \begin{array}{l} \mathbf{x} = x^i \mathbf{e}_i \\ \mathbf{y} = y^j \mathbf{e}_j \end{array} \right\} \quad \Longrightarrow \quad \mathbf{x} \bigwedge \mathbf{y} = (x^i y^j - y^i x^j)\,\mathbf{e}_i \otimes \mathbf{e}_j.$$

The components $p^{ij} = x^i y^j - y^i x^j$ of this tensor satisfy the properties

$$p^{ij} = -p^{ji}; \quad p^{ii} = 0.$$

It is an *antisymmetric* tensor of rank 2.

1.1.3.7.2. *Vector product*

Consider the so-called permutation tensor of rank 3 (it is actually an axial tensor – see Section 1.1.4.5.3) defined by

$$\begin{cases} \varepsilon_{ijk} = +1 & \text{if the permutation } ijk \text{ is even} \\ \varepsilon_{ijk} = -1 & \text{if the permutation } ijk \text{ is odd} \\ \varepsilon_{ijk} = 0 & \text{if at least two of the three indices are equal} \end{cases}$$

and let us form the contracted product

$$z_k = \tfrac{1}{2}\varepsilon_{ijk}p^{ij} = \varepsilon_{ijk}x^i y^j. \qquad (1.1.3.4)$$

It is easy to check that

$$\begin{cases} z_1 = x^2 y^3 - y^2 x^3 \\ z_2 = x^3 y^1 - y^3 x^1 \\ z_3 = x^1 y^2 - y^2 x^1. \end{cases}$$

One recognizes the coordinates of the vector product.

1.1.3.7.3. *Properties of the vector product*

Expression (1.1.3.4) of the vector product shows that it is of a covariant nature. This is indeed correct, and it is well known that the vector product of two vectors of the direct lattice is a vector of the reciprocal lattice [see Section 1.1.4 of Volume B of *International Tables for Crystallography* (2000)].

The vector product is a very particular vector which it is better not to call a vector: sometimes it is called a *pseudovector* or an *axial* vector in contrast to normal vectors or *polar* vectors. The components of the vector product are the independent components of the antisymmetric tensor p_{ij}. In the space of n dimensions, one would write

$$v_{i_3 i_4 \ldots i_n} = \tfrac{1}{2}\varepsilon_{i_1 i_2 \ldots i_n}p^{i_1 i_2}.$$

The number of independent components of p^{ij} is equal to $(n^2 - n)/2$ or 3 in the space of three dimensions and 6 in the space of four dimensions, and the independent components of p^{ij} are not the components of a vector in the space of four dimensions.

Let us also consider the behaviour of the vector product under the change of axes represented by the matrix

$$\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}.$$

This is a symmetry with respect to a point that transforms a right-handed set of axes into a left-handed set and reciprocally. In such a change, the components of a normal vector change sign. Those of the vector product, on the contrary, remain unchanged, indicating – as one well knows – that the orientation of the vector product has changed and that it is not, therefore, a vector in the normal sense, *i.e.* independent of the system of axes.

1.1.3.8. *Tensor derivatives*

1.1.3.8.1. *Interpretation of the coefficients of the matrix – change of coordinates*

We have under a change of axes:

$$x'^i = A^i_j x^j.$$

This shows that the new components, x'^i, can be considered linear functions of the old components, x^j, and one can write

$$A^i_j = \partial x'^i / \partial x^j = \partial_j x'^i.$$

It should be noted that the covariance has been increased.

1.1.3.8.2. *Generalization*

Consider a field of tensors t^j_i that are functions of space variables. In a change of coordinate system, one has

$$t^j_i = A^\alpha_i B^j_\beta t'^\beta_\alpha.$$

Differentiate with respect to x^k:

$$\frac{\partial t^j_i}{\partial x^k} = \partial_k t^j_i = A^\alpha_i B^j_\beta \frac{\partial t'^\beta_\alpha}{\partial x'^\gamma}\frac{\partial x'^\gamma}{\partial x^k}$$

$$\partial_k t^j_i = A^\alpha_i B^j_\beta A^\gamma_k \partial_\gamma t'^\beta_\alpha.$$

It can be seen that the partial derivatives $\partial_k t^j_i$ behave under a change of axes like a tensor of rank 3 whose covariance has been increased by 1 with respect to that of the tensor t^j_i. It is therefore possible to introduce a tensor of rank 1, ∇ (nabla), of which the components are the operators given by the partial derivatives $\partial/\partial x^i$.

1.1.3.8.3. *Differential operators*

If one applies the operator nabla to a scalar φ, one obtains

$$\text{grad } \varphi = \nabla\varphi.$$

This is a covariant vector in reciprocal space.

Now let us form the tensor product of ∇ by a vector $\mathbf{v}$ of variable components. We then have

$$\nabla \otimes \mathbf{v} = \frac{\partial v^j}{\partial x^i}\mathbf{e}_i \otimes \mathbf{e}^j.$$

The quantities $\partial_i v^j$ form a tensor of rank 2. If we contract it, we obtain the divergence of $\mathbf{v}$:

$$\text{div } \mathbf{v} = \partial_i v^i.$$

Taking the vector product, we get

$$\text{curl } \mathbf{v} = \nabla \wedge \mathbf{v}.$$

The curl is then an axial vector.

1.1.3.8.4. *Development of a vector function in a Taylor series*

Let $\mathbf{u(r)}$ be a vector function. Its development as a Taylor series is written

$$u^i(\mathbf{r} + \mathrm{d}\mathbf{r}) = u^i(\mathbf{r}) + \frac{\partial u^i}{\partial x^j}\,\mathrm{d}x^j + \tfrac{1}{2}\frac{\partial^2 u^i}{\partial x^j \partial x^k}\,\mathrm{d}x^j\,\mathrm{d}x^k + \ldots. \quad (1.1.3.5)$$

The coefficients of the expansion, $\partial u^i/\partial x^j$, $\partial^2 u^i/\partial x^j \partial x^k, \ldots$ are tensors of rank 2, 3, ...

An example is given by the relation between displacement and electric field:

$$D^i = \varepsilon^i_j E^j + \chi^i_{jk} E^j E^k + \ldots$$

(see Sections 1.6.2 and 1.7.2).

We see that the linear relation usually employed is in reality a development that is arrested at the first term. The second term corresponds to nonlinear optics. In general, it is very small but is not negligible in ferroelectric crystals in the neighbourhood of the ferroelectric–paraelectric transition. Nonlinear optics are studied in Chapter 1.7.

1.1.4. Symmetry properties

For the symmetry properties of the tensors used in physics, the reader may also consult Bhagavantam (1966), Billings (1969), Mason (1966), Nowick (1995), Nye (1985), Paufler (1986), Shuvalov (1988), Sirotin & Shaskol'skaya (1982), and Wooster (1973).

1.1.4.1. *Introduction – Neumann's principle*

We saw in Section 1.1.1 that physical properties express in general the response of a medium to an impetus. It has been known for a long time that symmetry considerations play an important role in the study of physical phenomena. These considerations are often very fruitful and have led, for instance, to the discovery of piezoelectricity by the Curie brothers in 1880 (Curie & Curie, 1880, 1881). It is not unusual for physical properties to be related to asymmetries. This is the case in electrical polarization, optical activity *etc.* The first to codify this role was the German physicist and crystallographer F. E. Neumann, who expressed in 1833 the *symmetry principle*, now called *Neumann's principle*: *if a crystal is invariant with respect to certain symmetry elements, any of its physical properties must also be invariant with respect to the same symmetry elements* (Neumann, 1885).

This principle may be illustrated by considering the optical properties of a crystal. In an anisotropic medium, the index of refraction depends on direction. For a given wave normal, two waves may propagate, with different velocities; this is the double refraction effect. The indices of refraction of the two waves vary with direction and can be found by using the index ellipsoid known as the *optical indicatrix* (see Section 1.6.3.2). Consider the central section of the ellipsoid perpendicular to the direction of propagation of the wave. It is an ellipse. The indices of the two waves that may propagate along this direction are equal to the semi-axes of that ellipse. There are two directions for which the central section is circular, and therefore two wave directions for which there is no double refraction. These directions are called optic axes, and the medium is said to be *biaxial*. If the medium is invariant with respect to a threefold, a fourfold or a sixfold axis (as in a trigonal, tetragonal or hexagonal crystal, for instance), its ellipsoid must also be invariant with respect to the same axis, according to Neumann's principle. As an ellipsoid can only be ordinary or of revolution, the indicatrix of a trigonal, tetragonal or hexagonal crystal is necessarily an ellipsoid of revolution that has only one circular central section and one optic axis. These crystals are said to be *uniaxial*. In a cubic crystal that has four threefold axes, the indicatrix must have several axes of revolution, it is therefore a sphere, and cubic media behave as isotropic media for properties represented by a tensor of rank 2.

1.1.4.2. *Curie laws*

The example given above shows that the symmetry of the property may possess a higher symmetry than the medium. The property is represented in that case by the indicatrix. The symmetry of an ellipsoid is

$$\frac{A_2}{M}\frac{A_2'}{M'}\frac{A_2''}{M''}C = mmm \text{ for any ellipsoid}$$

(orthorhombic symmetry)

$$\frac{A_\infty}{M}\frac{\infty A_2}{\infty M}C = \frac{\infty}{m}m \text{ for an ellipsoid of revolution}$$

(cylindrical symmetry)

$$\infty\frac{A_\infty}{M}C = \infty\frac{\infty}{m} \text{ for a sphere}$$

(spherical symmetry).

[Axes A_∞ are axes of revolution, or *axes of isotropy*, introduced by Curie (1884, 1894), *cf. International Tables for Crystallography* (2002), Vol. A, Table 10.1.4.2.]

The symmetry of the indicatrix is identical to that of the medium if the crystal belongs to the orthorhombic holohedry and is higher in all other cases.

This remark is the basis of the generalization of the symmetry principle by P. Curie (1859–1906). He stated that (Curie, 1894):

(i) *the symmetry characteristic of a phenomenon is the highest compatible with the existence of the phenomenon*;

(ii) *the phenomenon may exist in a medium that possesses that symmetry or that of a subgroup of that symmetry*;

and concludes that some symmetry elements may coexist with the phenomenon but that their presence is not necessary. On the contrary, what is necessary is the *absence* of certain symmetry elements: 'asymmetry creates the phenomenon' ('*C'est la dissymétrie qui crée le phénomène*'; Curie, 1894, p. 400). Noting that physical phenomena usually express relations between a cause and an effect (an influence and a response), P. Curie restated the two above propositions in the following way, now known as Curie laws, although they are not, properly speaking, laws:

(i) *the asymmetry of the effects must pre-exist in the causes*;

(ii) *the effects may be more symmetric than the causes*.

The application of the Curie laws enable one to determine the symmetry characteristic of a phenomenon. Let us consider the phenomenon first as an effect. If Φ is the symmetry of the phenomenon and C the symmetry of the cause that produces it,

$$C \leq \Phi.$$

Let us now consider the phenomenon as a cause producing a certain effect with symmetry E:

$$\Phi \leq E.$$

We can therefore conclude that

$$C \leq \Phi \leq E.$$

If we choose among the various possible causes the most symmetric one, and among the various possible effects the one with the lowest symmetry, we can then determine the symmetry that characterizes the phenomenon.

As an example, let us determine the symmetry associated with a mechanical force. A force can be considered as the result of a traction effort, the symmetry of which is $A_\infty\infty M$. If considered as a cause, its effect may be the motion of a sphere in a given direction (for example, a spherical ball falling under its own weight). Again, the symmetry is $A_\infty\infty M$. The symmetries associated with the force considered as a cause and as an effect being the same, we may conclude that $A_\infty\infty M$ is its characteristic symmetry.

1.1.4.3. *Symmetries associated with an electric field and with magnetic induction (flux density)*

1.1.4.3.1. *Symmetry of an electric field*

Considered as an effect, an electric field may have been produced by two circular coaxial electrodes, the first one carrying positive electric charges, the other one negative charges (Fig. 1.1.4.1). The cause possesses an axis of revolution and an infinity of mirrors parallel to it, $A_\infty\infty M$. Considered as a cause, the electric field induces for instance the motion of a spherical electric charge parallel to itself. The associated symmetry is the same in each case, and the symmetry of the electric field is identical to that of a force, $A_\infty\infty M$. The electric polarization or the electric displacement have the same symmetry.
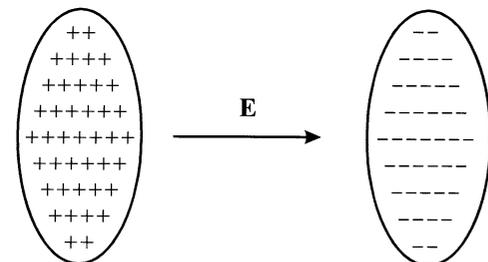

Fig. 1.1.4.1. Symmetry of an electric field.

1.1.4.3.2. *Symmetry of magnetic induction*

The determination of the symmetry of magnetic quantities is more delicate. Considered as an effect, magnetic induction may be obtained by passing an electric current in a loop (Fig. 1.1.4.2). The corresponding symmetry is that of a cylinder rotating around its axis, $(A_\infty/M)C$. Conversely, the variation of the flux of magnetic induction through a loop induces an electric current in the loop. If the magnetic induction is considered as a cause, its effect has the same symmetry. The symmetry associated with the magnetic induction is therefore $(A_\infty/M)C$.

This symmetry is completely different from that of the electric field. This difference can be understood by reference to Maxwell's equations, which relate electric and magnetic quantities:

$$\text{curl } \mathbf{E} = \nabla \wedge \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}; \quad \text{curl } \mathbf{H} = \nabla \wedge \mathbf{H} = \frac{\partial \mathbf{D}}{\partial t}.$$

It was seen in Section 1.1.3.8.3 that the curl is an axial vector because it is a vector product. Maxwell's equations thus show that if the electric quantities ($\mathbf{E}$, $\mathbf{D}$) are polar vectors, the magnetic quantities ($\mathbf{B}$, $\mathbf{H}$) are axial vectors and *vice versa*; the equations of Maxwell are, in effect, perfectly symmetrical on this point. Indeed, one could have been tempted to determine the symmetry of the magnetic field by considering interactions between magnets, which would have led to the symmetry $A_\infty\infty M$ for the magnetic quantities. However, in the world where we live and where the origin of magnetism is in the spin of the electron, the magnetic field is an axial vector of symmetry $(A_\infty/M)C$ while the electric field is a polar vector of symmetry $A_\infty\infty M$.

1.1.4.4. *Superposition of several causes in the same medium – pyroelectricity and piezolectricity*

1.1.4.4.1. *Introduction*

Let us now consider a phenomenon resulting from the superposition of several causes in the same medium. The symmetry of the global cause is the intersection of the groups of symmetry of the various causes: the asymmetries add up (Curie, 1894). This remark can be applied to the determination of the point groups where physical properties such as pyroelectricity or piezoelectricity are possible.

1.1.4.4.2. *Pyroelectricity*

Pyroelectricity is the property presented by certain materials that exhibit electric polarization when the temperature is changed uniformly. Actually, this property appears in crystals for which the centres of gravity of the positive and negative charges do not coincide in the unit cell. They present therefore a spontaneous polarization that varies with temperature because, owing to thermal expansion, the distances between these centres of gravity are temperature dependent. A very important case is that of the ferroelectric crystals where the direction of the polarization can be changed under the application of an external electric field.

From the viewpoint of symmetry, pyroelectricity can be considered as the superposition of two causes, namely the crystal

B
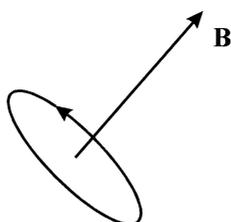
Fig. 1.1.4.2. Symmetry of magnetic induction.

with its symmetry on one hand and the increase of temperature, which is isotropic, on the other. The intersection of the groups of symmetry of the two causes is in this case identical to the group of symmetry of the crystal. The symmetry associated with the effect is that of the electric polarization that is produced, $A_\infty\infty M$. Since the asymmetry of the cause must pre-exist in the causes, the latter may not possess more than one axis of symmetry nor mirrors other than those parallel to the single axis. The only crystal point groups compatible with this condition are

$$1, 2, 3, 4, 6, m, 2mm, 3m, 4mm, 6mm.$$

There are therefore only ten crystallographic groups that are compatible with the pyroelectric effect. For instance, tourmaline, in which the effect was first observed, belongs to $3m$.

1.1.4.4.3. *Piezoelectricity*

Piezoelectricity, discovered by the Curie brothers (Curie & Curie, 1880), is the property presented by certain materials that exhibit an electric polarization when submitted to an applied mechanical stress such as a uniaxial compression (see, for instance, Cady, 1964; Ikeda, 1990). Conversely, their shape changes when they are submitted to an external electric field; this is the converse piezoelectric effect. The physical interpretation of piezoelectricity is the following: under the action of the applied stress, the centres of gravity of negative and positive charges move to different positions in the unit cell, which produces an electric polarization.

From the viewpoint of symmetry, piezoelectricity can be considered as the superposition of two causes, the crystal with its own symmetry and the applied stress. The symmetry associated with a uniaxial compression is that of two equal and opposite forces, namely $A_\infty/M \ \infty A_2/\infty MC$. The effect is an electric polarization, of symmetry $A_\infty\infty M$, which must be higher than or equal to the intersection of the symmetries of the two causes:

$$\frac{A_\infty}{M}\frac{\infty A_2}{\infty M}C\bigcap S_{\text{crystal}} \leq A_\infty\infty M,$$

where S_{crystal} denotes the symmetry of the crystal.

It may be noted that the effect does not possess a centre of symmetry. The crystal point groups compatible with the property of piezoelectricity are therefore among the 21 noncentrosymmetric point groups. More elaborate symmetry considerations show further that group 432 is also not compatible with piezoelectricity. This will be proved in Section 1.1.4.10.4 using the symmetry properties of tensors. There are therefore 20 point groups compatible with piezoelectricity:

$$1, \ 2, \ m, \ 222, \ 2mm,$$

$$3, \ 32, \ 3m, \ 4, \ \bar{4}, \ 422, \ 4mm, \ \bar{4}2m, \ 6, \ \bar{6}, \ 622, \ 6mm, \ \bar{6}2m$$

$$23, \ \bar{4}3m.$$

The intersection of the symmetries of the crystal and of the applied stress depend of course on the orientation of this stress relative to the crystallographic axes. Let us take, for instance, a crystal of quartz, which belongs to group $32 = A_3 3A_2$. The above condition becomes

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

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 dieletric constant tensor, ε_{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 9×9 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 $A = (T - T^T)/2$.

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 satifies 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

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

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 θ is the rotation angle of the light wave, d the distance traversed in the material and ρ 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

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

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

$$
c_{ijkl}(\omega, \mathbf{k}) = c_{ijkl}(\omega) + \mathrm{i}d_{ijklm}(\omega)k_m + \ldots,
$$

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

1.1.4.6.1. *Matrix method – application of Neumann's principle*

An operation of symmetry turns back the crystalline edifice on itself; it allows the physical properties of the crystal and the tensors representing them to be invariant. An operation of symmetry is equivalent to a change of coordinate system. In a change of system, a tensor becomes

$$
t'^{\alpha\beta}_{\gamma\delta} = t^{ij}_{kl}A^\alpha_i A^\beta_j B^k_\gamma B^l_\delta.
$$

If A represents a symmetry operation, it is a unitary matrix:

$$A = B^T = B^{-1}.$$

Since the tensor is invariant under the action of the symmetry operator A, one has, according to Neumann's principle,

$$t'^{\alpha\beta}_{\gamma\delta} = t^{\alpha\beta}_{\gamma\delta}$$

and, therefore,

$$t^{\alpha\beta}_{\gamma\delta} = t^{ij}_{kl} A^{\alpha}_i A^{\beta}_j B^k_\gamma B^l_\delta. \qquad (1.1.4.1)$$

There are therefore a certain number of linear relations between the components of the tensor and the number of independent components is reduced. If there are p components and q relations between the components, there are $p - q$ independent components. This number is *independent* of the system of axes. When applied to each of the 32 point groups, this reduction enables one to find the form of the tensor in each case. It depends on the rank of the tensor. In the present chapter, the reduction will be derived for tensors up to the fourth rank and for all crystallographic groups as well as for the isotropic groups. An orthonormal frame will be assumed in all cases, so that co- and contravariance will not be apparent and the positions of indices as subscripts or superscripts will not be meaningful. The Ox_3 axis will be chosen parallel to the threefold, fourfold or sixfold axis in the trigonal, tetragonal and hexagonal systems. The accompanying software to the present volume enables the reduction for tensors of any rank to be derived.

1.1.4.6.2. *The operator A is in diagonal form*

1.1.4.6.2.1. *Introduction*

If one takes as the system of axes the eigenvectors of the operator A, the matrix is written in the form

$$\begin{pmatrix} \exp i\theta & 0 & 0 \\ 0 & \exp -i\theta & 0 \\ 0 & 0 & \pm 1 \end{pmatrix},$$

where θ is the rotation angle, Ox_3 is taken parallel to the rotation axis and coefficient A_3 is equal to +1 or −1 depending on whether the rotation axis is direct or inverse (proper or improper operator).

The equations (1.1.4.1) can then be simplified and reduce to

$$t^{ij}_{kl} = t^{ij}_{kl} A^{\alpha}_i A^{\beta}_j B^k_\gamma B^l_\delta \qquad (1.1.4.2)$$

(*without* any summation).

If the product $A^i_i A^j_j B^k_k B^l_l$ (without summation) is equal to unity, equation (1.1.4.2) is trivial and there is significance in the component t_{kl}. On the contrary, if it is different from 1, the only solution for (1.1.4.2) is that $t^{ij}_{kl} = 0$. One then finds immediately that certain components of the tensor are zero and that others are unchanged.

1.1.4.6.2.2. *Case of a centre of symmetry*

All the diagonal components are in this case equal to −1. One thus has:

(i) *Tensors of even rank*, $t^{ij\cdots} = (-1)^{2p} t^{ij\cdots}$. The components are not affected by the presence of the centre of symmetry. The reduction of tensors of even rank is therefore the same in a centred group and in its noncentred subgroups, that is in any of the 11 *Laue classes*:

$\bar{1}$	1
$2/m$	2, m
mmm	222, 2mm
$\bar{3}$	3
$\bar{3}m$	32, 3m
$4/m$	$\bar{4}$, 4
$4/mm$	$\bar{4}2m$, 422, 4mm
$6/m$	$\bar{6}$, 6
$6/mm$	$\bar{6}2m$, 622, 6mm
$m\bar{3}$	23
$m\bar{3}m$	432, $\bar{4}32$.

If a tensor is invariant with respect to two elements of symmetry, it is invariant with respect to their product. It is then sufficient to make the reduction for the generating elements of the group and (since this concerns a tensor of even rank) for the 11 *Laue classes*.

(ii) *Tensors of odd rank*, $t^{ij\cdots} = (-1)^{2p+1} t^{ij\cdots}$. *All* the components are equal to zero. The physical properties represented by tensors of rank 3, such as piezoelectricity, piezomagnetism, nonlinear optics, for instance, will therefore not be present in a centrosymmetric crystal.

1.1.4.6.2.3. *General case*

By replacing the matrix coefficients A^i_i by their expression, (1.1.4.2) becomes, for a proper rotation,

$$t^{jk\cdots} = t^{jk\cdots} \exp(ir\theta) \exp(-is\theta)(1)^t = t^{jk\cdots} \exp i(r - s)\theta,$$

where r is the number of indices equal to 1, s is the number of indices equal to 2, t is the number of indices equal to 3 and $r + s + t = p$ is the rank of the tensor. The component $t^{jk\cdots}$ is not affected by the symmetry operation if

$$(r - s)\theta = 2K\pi,$$

where K is an integer, and is equal to zero if

$$(r - s)\theta \neq 2K\pi.$$

The angle of rotation θ can be put into the form $2\pi/q$, where q is the order of the axis. The condition for the component not to be zero is then

$$r - s = Kq.$$

The condition is fulfilled differently depending on the rank of the tensor, p, and the order of the axis, q. Indeed, we have $r - s \leq p$ and

$p = 2, r - s \leq 2$: *the result of the reduction will be the same for any* $q \geq 3$;

$p = 3, r - s \leq 3$: *the result of the reduction will be the same for any* $q \geq 4$;

$p = 4, r - s \leq 4$: *the result of the reduction will be the same for any* $q \geq 5$.

It follows that:

(i) for tensors of rank 2, the reduction will be the same for trigonal (threefold axis), tetragonal (fourfold axis) and hexagonal (sixfold axis) groups;

(ii) for tensors of rank 3, the reduction will be the same for tetragonal and hexagonal groups;

(iii) for tensors of rank 4, the reduction will be different for trigonal, tetragonal and hexagonal groups.

The inconvenience of the diagonalization method is that the vectors and eigenvalues are, in general, complex, so in practice one uses another method. For instance, we may note that equation (1.1.4.1) can be written in the case of $p = 2$ by associating with the tensor a 3×3 matrix T:

$$T = BTB^T,$$

where B is the symmetry operation. Through identification of homologous coefficients in matrices T and BTB^T, one obtains relations between components t_{ij} that enable the determination of the independent components.

1.1.4.6.3. *The method of direct inspection*

The method of 'direct inspection', due to Fumi (1952*a,b*, 1987), is very simple. It is based on the fundamental properties of tensors; the components transform under a change of basis like a product of vector components (Section 1.1.3.2).

Examples

(1) Let us consider a tensor of rank 3 invariant with respect to a twofold axis parallel to Ox_3. The matrix representing this operator is

$$\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

The component t_{ijk} behaves under a change of axes like the product of the components x_i, x_j, x_k. The components x_1, x_2, x_3 of a vector become, respectively, $-x_1, -x_2, x_3$. To simplify the notation, we shall denote the components of the tensor simply by ijk. If, amongst the indices i, j and k, there is an even number (*including the number zero*) of indices that are equal to 3, the product $x_i x_j x_k$ will become $-x_i x_j x_k$ under the rotation. As the component 'ijk' remains invariant and is also equal to its opposite, it must be zero. 14 components will thus be equal to zero:

111, 122, 133, 211, 222, 133, 112, 121, 212, 221, 323, 331, 332, 313.

(2) Let us now consider that the same tensor of rank 3 is invariant with respect to a fourfold axis parallel to Ox_3. The matrix representing this operator and its action on a vector of coordinates x_1, x_2, x_3 is given by

$$\begin{pmatrix} x_2 \\ -x_1 \\ x_3 \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}. \qquad (1.1.4.3)$$

Coordinate x_1 becomes x_2, x_2 becomes $-x_1$ and x_3 becomes x_3. Component ijk transforms like product $x^i x^j x^k$ according to the rule given above. Since the twofold axis parallel to Ox_3 is a subgroup of the fourfold axis, we can start from the corresponding reduction. We find

$$
\begin{array}{llll}
311 & \Longleftrightarrow & 322 & : \quad t_{311} = \quad t_{322} \\
123 & \Longleftrightarrow & -(213) & : \quad t_{123} = \quad -t_{213} \\
113 & \Longleftrightarrow & 223 & : \quad t_{113} = \quad t_{223} \\
333 & \Longleftrightarrow & 333 & : \quad t_{333} = \quad t_{333} \\
132 & \Longleftrightarrow & -(231) & : \quad t_{132} = \quad -t_{231} \\
131 & \Longleftrightarrow & 232 & : \quad t_{131} = \quad t_{232} \\
312 & \Longleftrightarrow & -(321) & : \quad t_{312} = \quad -t_{321}.
\end{array}
$$

All the other components are equal to zero.

It is not possible to apply the method of direct inspection for point group 3. One must in this case use the matrix method described in Section 1.1.4.6.2; once this result is assumed, the method can be applied to all other point groups.

1.1.4.7. *Reduction of the components of a tensor of rank 2*

The reduction is given for each of the 11 Laue classes.

1.1.4.7.1. *Triclinic system*

Groups $\bar{1}$, 1: no reduction, the tensor has 9 independent components. The result is represented in the following symbolic way (Nye, 1957, 1985):

where the sign $\bullet$ represents a nonzero component.

1.1.4.7.2. *Monoclinic system*

Groups 2*m*, 2, *m*: it is sufficient to consider the twofold axis or the mirror. As the representative matrix is diagonal, the calculation is immediate. Taking the twofold axis to be parallel to Ox_3, one has

$$t_3^1 = t_1^3 = t_3^2 = t_2^3 = 0.$$

The other components are not affected. The result is represented as

There are 5 independent components. If the twofold axis is taken along axis Ox_2, which is the usual case in crystallography, the table of independent components becomes

1.1.4.7.3. *Orthorhombic system*

Groups *mmm*, 2*mm*, 222: the reduction is obtained by considering two perpendicular twofold axes, parallel to Ox_3 and to Ox_2, respectively. One obtains

There are 3 independent components.

1.1.4.7.4. *Trigonal, tetragonal, hexagonal and cylindrical systems*

We remarked in Section 1.1.4.6.2.3 that, in the case of tensors of rank 2, the reduction is the same for threefold, fourfold or sixfold axes. It suffices therefore to perform the reduction for the tetragonal groups. That for the other systems follows automatically.

1.1.4.7.4.1. *Groups* $\bar{3}$, 3; 4/*m*, $\bar{4}$, 4; 6/*m*, $\bar{6}$, 6; $(A_\infty/M)C$, A_∞

If we consider a fourfold axis parallel to Ox_3 represented by the matrix given in (1.1.4.3), by applying the direct inspection method one finds

where the symbol $\ominus$ means that the corresponding component is numerically equal to that to which it is linked, but of opposite sign. There are 3 independent components.

1.1.4.7.4.2. Groups $\bar{3}m$, 32, 3m; 4/mm, 422, 4mm, $\bar{4}2m$; 6/mm, 622, 6mm, $\bar{6}2m$; $(A_\infty/M)\infty(A_2/M)C$, $A_\infty\infty A_2$

The result is obtained by combining the preceding result and that corresponding to a twofold axis normal to the fourfold axis. One finds

$$\begin{pmatrix} \bullet & & \\ & \bullet & \\ & & \bullet \end{pmatrix}$$
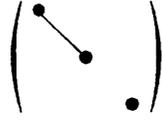
There are 2 independent components.

1.1.4.7.5. *Cubic and spherical systems*

The cubic system is characterized by the presence of threefold axes along the $\langle 111 \rangle$ directions. The action of a threefold axis along [111] on the components x_1, x_2, x_3 of a vector results in a permutation of these components, which become, respectively, x_2, x_3, x_1 and then x_3, x_1, x_2. One deduces that the components of a tensor of rank 2 satisfy the relations

$$t_1^1 = t_2^2 = t_3^3.$$

The cubic groups all include as a subgroup the group 23 of which the generating elements are a twofold axis along Ox_3 and a threefold axis along [111]. If one combines the corresponding results, one deduces that

$$t_1^2 = t_2^3 = t_3^1 = t_1^3 = t_2^1 = t_3^2 = 0,$$

which can be summarized by

$$\begin{pmatrix} \bullet & & \\ & \bullet & \\ & & \bullet \end{pmatrix}$$
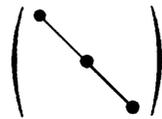
There is a single independent component and the medium behaves like a property represented by a tensor of rank 2, like an isotropic medium.

1.1.4.7.6. *Symmetric tensors of rank 2*

If the tensor is symmetric, the number of independent components is still reduced. One obtains the following, representing the nonzero components for the leading diagonal and for one half of the others.

1.1.4.7.6.1. *Triclinic system*

$$\begin{pmatrix} \bullet & \bullet & \bullet \\ & \bullet & \bullet \\ & & \bullet \end{pmatrix}$$
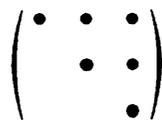
There are 6 independent components. It is possible to interpret the number of independent components of a tensor of rank 2 by considering the associated quadric, for instance the optical indicatrix. In the triclinic system, the quadric is any quadric. It is characterized by six parameters: the lengths of the three axes and the orientation of these axes relative to the crystallographic axes.

1.1.4.7.6.2. *Monoclinic system (twofold axis parallel to Ox_2)*

$$\begin{pmatrix} \bullet & & \bullet \\ & \bullet & \\ \bullet & & \bullet \end{pmatrix}$$
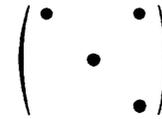
There are 4 independent components. The quadric is still any quadric, but one of its axes coincides with the twofold axis of the monoclinic lattice. Four parameters are required: the lengths of the axes and one angle.

1.1.4.7.6.3. *Orthorhombic system*

$$\begin{pmatrix} \bullet & & \\ & \bullet & \\ & & \bullet \end{pmatrix}$$

There are 3 independent components. The quadric is any quadric, the axes of which coincide with the crystallographic axes. Only three parameters are required.

1.1.4.7.6.4. *Trigonal, tetragonal and hexagonal systems, isotropic groups*

$$\begin{pmatrix} \bullet & & \\ & \bullet & \\ & & \bullet \end{pmatrix}$$
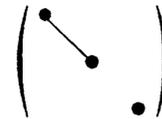
There are 2 independent components. The quadric is of revolution. It is characterized by two parameters: the lengths of its two axes.

1.1.4.7.6.5. *Cubic system*

$$\begin{pmatrix} \bullet & & \\ & \bullet & \\ & & \bullet \end{pmatrix}$$

There is 1 independent component. The associated quadric is a sphere.

1.1.4.8. *Reduction of the components of a tensor of rank 3*

1.1.4.8.1. *Triclinic system*

1.1.4.8.1.1. *Group* 1

All the components are independent. Their number is equal to 27. They are usually represented as a 3×9 matrix which can be subdivided into three 3×3 submatrices:

$$\begin{pmatrix} 111 & 122 & 133 & 123 & 131 & 112 & 132 & 113 & 121 \\ 211 & 222 & 233 & 223 & 231 & 212 & 232 & 213 & 221 \\ 311 & 322 & 333 & 323 & 331 & 312 & 332 & 313 & 321 \end{pmatrix}.$$

1.1.4.8.1.2. *Group* $\bar{1}$

All the components are equal to zero.

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1.1.4.8.2. Monoclinic system

1.1.4.8.2.1. Group 2

Choosing the twofold axis parallel to Ox_3 and applying the direct inspection method, one finds

There are 13 independent components. If the twofold axis is parallel to Ox_2, one finds

1.1.4.8.2.2. Group m

One obtains the matrix representing the operator m by multiplying by -1 the coefficients of the matrix representing a twofold axis. The result of the reduction will then be exactly complementary: the components of the tensor which include an odd number of 3's are now equal to zero. One writes the result as follows:

There are 14 independent components. If the mirror axis is normal to Ox_2, one finds

1.1.4.8.2.3. Group 2/m

All the components are equal to zero.

1.1.4.8.3. Orthorhombic system

1.1.4.8.3.1. Group 222

There are three orthonormal twofold axes. The reduction is obtained by combining the results associated with two twofold axes, parallel to Ox_3 and Ox_2, respectively.

There are 6 independent components.

1.1.4.8.3.2. Group mm2

The reduction is obtained by combining the results associated with a twofold axis parallel to Ox_3 and with a mirror normal to Ox_2:

There are 7 independent components.

1.1.4.8.3.3. Group mmm

All the components are equal to zero.

1.1.4.8.4. Trigonal system

1.1.4.8.4.1. Group 3

The threefold axis is parallel to Ox_3. The matrix method should be used here. One finds

There are 9 independent components.

1.1.4.8.4.2. Group 32 with a twofold axis parallel to Ox_1

There are 4 independent components.

1.1.4.8.4.3. Group 3m with a mirror normal to Ox_1

There are 4 independent components.

1.1.4.8.4.4. Groups $\bar{3}$ and $\bar{3}m$

All the components are equal to zero.

1.1.4.8.5. Tetragonal system

1.1.4.8.5.1. Group 4

The method of direct inspection can be applied for a fourfold axis. One finds
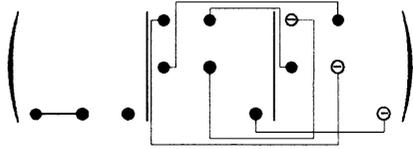
There are 7 independent components.

1.1.4.8.5.2. Group 422

One combines the reductions for groups 4 and 222:
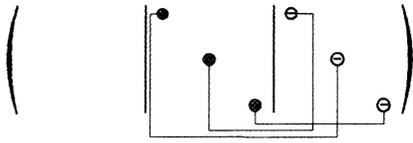
There are 3 independent components.

1.1.4.8.5.3. Group 4mm

One combines the reductions for groups 4 and 2m:
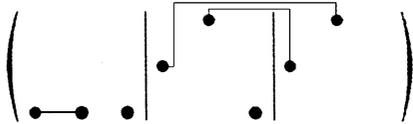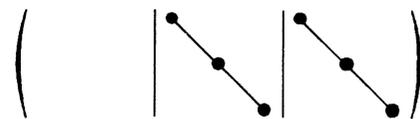
There are 4 independent components.

1.1.4.8.5.4. Group 4/m

All the components are equal to zero.

1.1.4.8.5.5. Group $\bar{4}$

The matrix corresponding to axis $\bar{4}$ is

$$\begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$$

and the form of the 3×9 matrix is
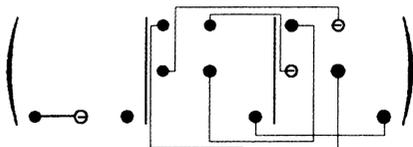
There are 6 independent components.

1.1.4.8.5.6. Group $\bar{4}2m$

One combines either the reductions for groups $\bar{4}$ and 222, or the reductions for groups $\bar{4}$ and 2mm.
(i) Twofold axis parallel to Ox_1:
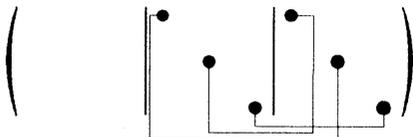
There are 6 independent components.

(ii) Mirror perpendicular to Ox_1 (the twofold axis is at 45°)
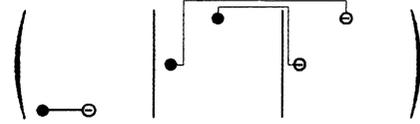
The number of independent components is of course the same, 6.

1.1.4.8.5.7. Group 4/mm

All the components are equal to zero.

1.1.4.8.6. Hexagonal and cylindrical systems

1.1.4.8.6.1. Groups 6, A_∞, 622, $A_\infty \infty A_2$, 6mm and $A_\infty \infty M$

It was shown in Section 1.1.4.6.2.3 that, in the case of tensors of rank 3, the reduction is the same for axes of order 4, 6 or higher. The reduction will then be the same as for the tetragonal system.

1.1.4.8.6.2. Group $\bar{6} = 3/m$

One combines the reductions for the groups corresponding to a threefold axis parallel to Ox_3 and to a mirror perpendicular to Ox_3:
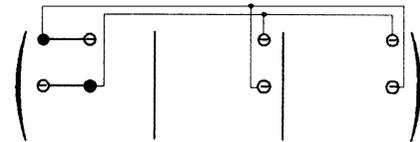
There are 2 independent components.

1.1.4.8.6.3. Group $\bar{6}2m$

One combines the reductions for groups 6 and 2mm:
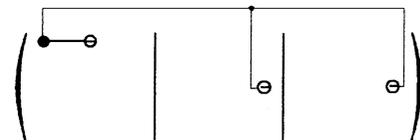
There is 1 independent component.

1.1.4.8.6.4. Groups 6/m, $(A_\infty/M)C$, 6/mm and $(A_\infty/M)\infty(A_2/M)C$

All the components are equal to zero.

1.1.4.8.7. Cubic and spherical systems

1.1.4.8.7.1. Group 23

One combines the reductions corresponding to a twofold axis parallel to Ox_3 and to a threefold axis parallel to [111]:

There are 2 independent components.

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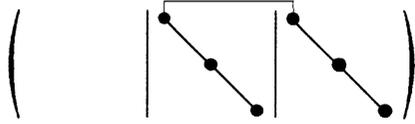#### 1.1.4.8.7.2. Groups 432 and $\infty A_\infty/M$

One combines the reductions corresponding to groups 422 and 23:
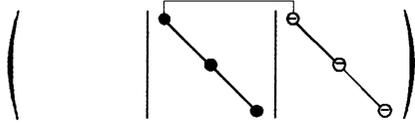
There is 1 independent component.

1.1.4.8.7.3. Group $\bar{4}3m$

One combines the reductions corresponding to groups $\bar{4}2m$ and 23:

There is 1 independent component.

1.1.4.8.7.4. Groups $m\bar{3}$, $m\bar{3}m$ and $\infty(A_\infty/M)C$

All the components are equal to zero.

1.1.4.9. Reduction of the components of a tensor of rank 4

1.1.4.9.1. Triclinic system (groups $\bar{1}$, 1)

There is no reduction; all the components are independent. Their number is equal to 81. They are usually represented as a 9×9 matrix, where components t_{ijkl} are replaced by $ijkl$, for brevity:

kl	11	22	33	23	31	12	32	13	21
ij									
11	1111	1122	1133	1123	1131	1112	1132	1113	1121
22	2211	2222	2233	2223	2231	2212	2232	2213	2221
33	3311	3322	3333	3323	3331	3312	3332	3313	3321
23	2311	2322	2333	2323	2331	2312	2332	2313	2321
31	3111	3122	3133	3123	3131	3112	3132	3113	3121
12	1211	1222	1233	1223	1231	1212	1232	1213	1221
32	3211	3222	3233	3223	3231	3212	3232	3213	3221
13	1311	1322	1333	1323	1331	1312	1332	1313	1321
21	2111	2122	2133	2123	2131	2112	2132	2113	2121

This matrix can be represented symbolically by
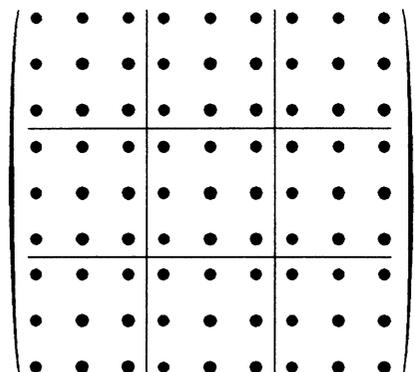
where the 9×9 matrix has been subdivided for clarity in to nine 3×3 submatrices.

1.1.4.9.2. Monoclinic system (groups $2/m$, 2, m)

The reduction is obtained by the method of direct inspection. For a twofold axis parallel to Ox_2, one finds
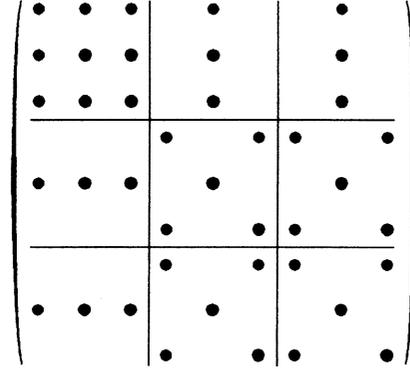
There are 41 independent components.

1.1.4.9.3. Orthorhombic system (groups mmm, 2mm, 222)
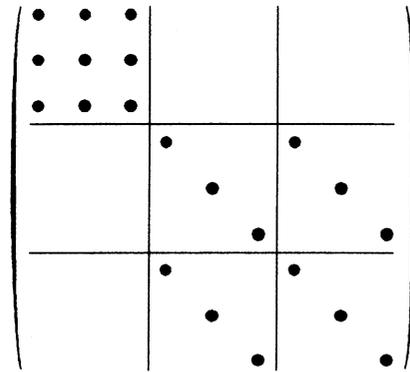
There are 21 independent components.

1.1.4.9.4. Trigonal system

1.1.4.9.4.1. Groups 3 and $\bar{3}$

The reduction is first applied in the system of axes tied to the eigenvectors of the operator representing a threefold axis. The system of axes is then changed to a system of orthonormal axes with Ox_3 parallel to the threefold axis:

kl	11	22	33	23	31	12	32	13	21
ij									
11	1111	1122	1133	1123	-2231	1112	1132	-2213	1121
22	1122	1111	1133	-1123	2231	-1121	-1132	2213	-1112
33	3311	3311	3333			3312			-3312
23	2311	-2311		2323	2331	1322	2332	2313	1322
31	-3122	3122		3123	3131	3211	3132	3113	3211
12	1211	-2111	1233	2213	1132	1212	2231	1123	1221
32	3211	-3211		3113	-3132	3122	3131	-3123	3122
13	-1322	1322		-2313	2332	2311	-2331	2323	2311
21	2111	-121	-1233	2213	1132	1221	2231	1123	1212

with

$$\left.\begin{array}{rl} t_{1111} - t_{1122} = & t_{1212} + t_{1221} \\ t_{1112} + t_{1121} = & -(t_{1211} + t_{2111}). \end{array}\right\}$$

There are 27 independent components.

1.1.4.9.4.2. Groups $\bar{3}m$, 32, 3m, with the twofold axis parallel to Ox_1

kl / ij	11	22	33	23	31	12	32	13	21
11	1111	1122	1133	1123			1132		
22	1122	1111	1133	−1123			−1132		
33	3311	3311	3333						
23	2311	−2311		2323			2332		
31					3131	3211		3113	3211
12					1132	1212		1123	1221
32	3211	−3211		3113			3131		
13					2332	2311		2323	2311
21					1132	1221		1123	1212

with

$$t_{1111} - t_{1122} = t_{1212} + t_{1221}.$$

There are 14 independent components.

1.1.4.9.5. Tetragonal system
1.1.4.9.5.1. Groups 4/m, 4, $\bar{4}$

kl / ij	11	22	33	23	31	12	32	13	21
11	1111	1122	1133			1112			−2212
22	1122	1111	1133			2212			−1112
33	3311	3311	3333			3312			−3312
23				2323	2331		2332	2313	
31				3123	3131		3132	3113	
12	1211	1222	1233			1212			1221
32				3113	−3132		3131	−3123	
13				−2313	2332		−2331	2323	
21	−1222	−1211	−1233						1212

There are 21 independent components.

1.1.4.9.5.2. Groups 4/mm, 422, 4mm, $\bar{4}2m$

kl / ij	11	22	33	23	31	12	32	13	21
11	1111	1122	1133						
22	1122	1111	1133						
33	3311	3311	3333						
23				2323			2332		
31					3131			3113	
12						1212			1221
32				3113			3131		
13					2332			2323	
21						1221			1212

There are 11 independent components.

1.1.4.9.6. Hexagonal and cylindrical systems
1.1.4.9.6.1. Groups 6/m, $\bar{6}$, 6; $(A_\infty/M)C$, A_∞

kl / ij	11	22	33	23	31	12	32	13	21
11	1111	1122	1133			1112			1121
22	1122	1111	1133			−1121			−1112
33	3311	3311	3333			3312			−3312
23				2323	2331		2332	2313	
31				3123	3131		3132	3113	
12	1211	−2111	1233			1212			1221
32				3113	−3132		3131	−3123	
13				−2313	2332		−2331	2323	
21	2111	−1211	−1233		1132	1221		1123	1212

with

$$\left.\begin{array}{l} t_{1111} - t_{1122} = t_{1212} + t_{1221} \\ t_{1112} + t_{1121} = -(t_{1211} + t_{2111}). \end{array}\right\}$$

There are 19 independent components.

1.1.4.9.6.2. Groups 6/mm, 622, 6mm, $\bar{6}2m$; $(A_\infty/M)\infty$; $(A_2/M)C$, $A_\infty\infty A_2$

kl / ij	11	22	33	23	31	12	32	13	21
11	1111	1122	1133						
22	1122	1111	1133						
33	3311	3311	3333						
23				2323			2332		
31					3131			3113	
12						1212			1221
32				3113			3131		
13					2332			2323	
21						1221			1212

with

$$t_{1111} - t_{1122} = t_{1212} + t_{1221}.$$

There are 11 independent components.

1.1.4.9.7. Cubic system
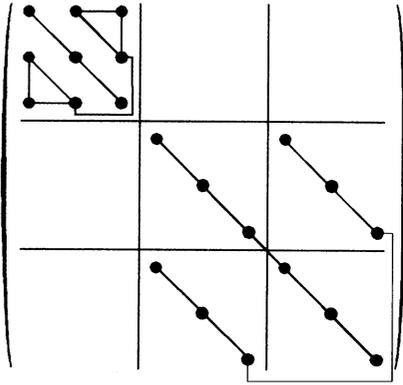### 1.1.4.9.7.1. Groups 23, $\bar{3}m$
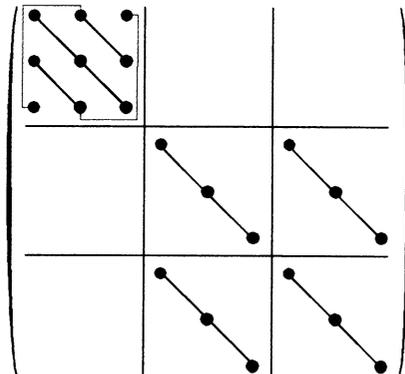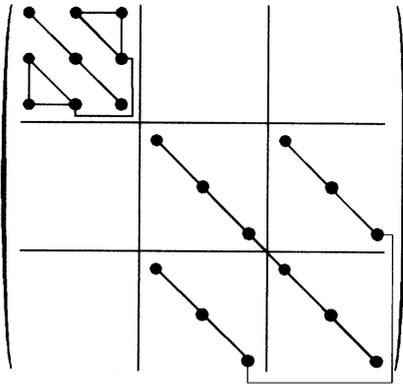
There are 7 independent components.

1.1.4.9.7.2. Groups $m\bar{3}m$, 432, $\bar{4}3m$

There are 4 independent components. The tensor is symmetric.

1.1.4.9.8. Spherical system
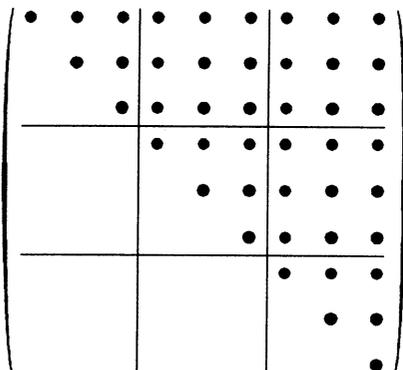### 1.1.4.9.8.1. Groups $\infty(A_\infty/M)C$ and ∞A_∞

with

$$t_{1111} - t_{1122} = t_{1212} + t_{1221}.$$

There are 3 independent components. The tensor is symmetric.
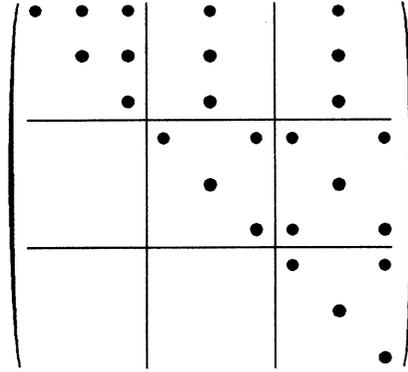
1.1.4.9.9. Symmetric tensors of rank 4

For symmetric tensors such as those representing principal properties, one finds the following, representing the nonzero components for the leading diagonal and for one half of the others.

1.1.4.9.9.1. Triclinic system

There are 45 independent coefficients.

1.1.4.9.9.2. Monoclinic system

There are 25 independent coefficients.

1.1.4.9.9.3. Orthorhombic system
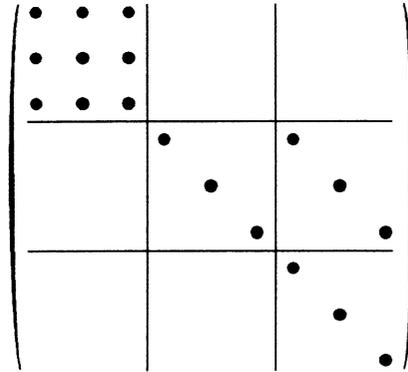
There are 15 independent coefficients.

1.1.4.9.9.4. Trigonal system
(i) Groups 3 and $\bar{3}$

$\begin{matrix}kl\\ij\end{matrix}$	11	22	33	23	31	12	32	13	21
11	1111	1122	1133	1123	−2231	1112	1132	−2213	−1112
22		1111	1133	−1123	2231	−1121	−1132	2213	−1112
33			3333			3312			−3312
23				2323	2331	2213	2332		2213
31					3131	1132		2332	1132
12						1212	2231	1123	1221
32							3131	−2331	2231
13								2323	1123
21									1212

with

$$t_{1111} - t_{1122} = t_{1212} + t_{1221}.$$

There are 15 independent components.

(ii) Groups $\bar{3}m$, 32, 3m

ij \ kl	11	22	33	23	31	12	32	13	21
11	1111	1122	1133	1123			1132		
22		1111	1133	−1123			−1132		
33			3333						
23				2323			2332		
31					3131	1132		2332	1132
12						1212		1123	1221
32							3131		
13								2323	1123
21									1212

with

$$t_{1111} - t_{1122} = t_{1212} + t_{1221}.$$

There are 11 independent components.

1.1.4.9.9.5. *Tetragonal system*

(i) Groups $4/m$, 4, $\bar{4}$

ij \ kl	11	22	33	23	31	12	32	13	21
11	1111	1122	1133			1112			−2212
22		1111	1133			2212			−1112
33			3333			3312			−3312
23				2323	2331		2332		
31					3131			2332	
12						1212			1221
32							3131	−2331	
13								2323	
21									1212

There are 13 independent components.

(ii) Groups $4/mm$, 422, 4mm, $\bar{4}2m$

ij \ kl	11	22	33	23	31	12	32	13	21
11	1111	1122	1133						
22		1111	1133						
33			3333						
23				2323			2332		
31					3131			3113	
12						1212			1221
32							3131		
13								2323	
21									1212

There are 9 independent components.

1.1.4.9.9.6. *Hexagonal and cylindrical systems*

(i) Groups $6/m$, $\bar{6}$, 6; $(A_\infty/M)C$, A_∞

ij \ kl	11	22	33	23	31	12	32	13	21
11	1111	1122	1133			1112			1121
22		1111	1133			−1121			−1112
33			3333			3312			−3312
23				2323	2331		2332		
31					3131		3132	2332	
12						1212			1221
32							3131	−2331	
13								2323	
21									1212

with

$$t_{1111} - t_{1122} = t_{1212} + t_{1221}.$$

There are 12 independent components.

(ii) Groups $6/mm$, 622, 6mm, $\bar{6}2m$; $(A_\infty/M)\infty(A_2/M)C$, $A_\infty\infty A_2$

ij \ kl	11	22	33	23	31	12	32	13	21
11	1111	1122	1133						
22		1111	1133						
33			3333						
23				2323			2332		
31					3131			3113	
12						1212			1221
32							3131		
13								2323	
21									1212

with

$$t_{1111} - t_{1122} = t_{1212} + t_{1221}.$$

There are 10 independent components.

1.1.4.9.9.7. *Cubic system*

(i) Groups 23, $\bar{3}m$

with

$$t_{1111} - t_{1122} = t_{1212} + t_{1221}.$$

There are 5 independent components.

(ii) Groups $m\bar{3}m$, 432, $\bar{4}3m$, and spherical system: the reduced tensors are already symmetric (see Sections 1.1.4.9.7 and 1.1.4.9.8).

1.1.4.10. *Reduced form of polar and axial tensors – matrix representation*

1.1.4.10.1. *Introduction*

Many tensors representing physical properties or physical quantities appear in relations involving symmetric tensors. Consider, for instance, the strain S_{ij} resulting from the application of an electric field **E** (the piezoelectric effect):

$$S_{ij} = d_{ijk}E_k + Q_{ijkl}E_kE_l, \qquad (1.1.4.4)$$

where the first-order terms d_{ijk} represent the components of the third-rank converse piezoelectric tensor and the second-order terms Q_{ijkl} represent the components of the fourth-rank electrostriction tensor. In a similar way, the direct piezoelectric effect corresponds to the appearance of an electric polarization **P** when a stress T_{jk} is applied to a crystal:

$$P_i = d_{ijk}T_{jk}. \qquad (1.1.4.5)$$

Owing to the symmetry properties of the strain and stress tensors (see Sections 1.3.1 and 1.3.2) and of the tensor product E_kE_l, there occurs a further reduction of the number of independent components of the tensors which are engaged in a contracted product with them, as is shown in Section 1.1.4.10.3 for third-rank tensors and in Section 1.1.4.10.5 for fourth-rank tensors.

1.1.4.10.2. *Stress and strain tensors – Voigt matrices*

The stress and strain tensors are symmetric because body torques and rotations are not taken into account, respectively (see Sections 1.3.1 and 1.3.2). Their components are usually represented using Voigt's one-index notation.

(i) Strain tensor

$$\left.\begin{array}{lll} S_1 = S_{11}; & S_2 = S_{22}; & S_3 = S_{33}; \\ S_4 = S_{23} + S_{32}; & S_5 = S_{31} + S_{13}; & S_6 = S_{12} + S_{21}; \\ S_4 = 2S_{23} = 2S_{32}; & S_5 = 2S_{31} = 2S_{13}; & S_6 = 2S_{12} = 2S_{21}. \end{array}\right\}$$
$$(1.1.4.6)$$

The Voigt components S_α form a Voigt matrix:

$$\begin{pmatrix} S_1 & S_6 & S_5 \\ & S_2 & S_4 \\ & & S_3 \end{pmatrix}.$$

The terms of the leading diagonal represent the elongations (see Section 1.3.1). It is important to note that the non-diagonal terms, which represent the shears, are here equal to *twice* the corresponding components of the strain tensor. The components S_α of the Voigt strain matrix are therefore *not* the components of a tensor.

(ii) Stress tensor

$$\left.\begin{array}{lll} T_1 = T_{11}; & T_2 = T_{22}; & T_3 = T_{33}; \\ T_4 = T_{23} = T_{32}; & T_5 = T_{31} = T_{13}; & T_6 = T_{12} = T_{21}. \end{array}\right\}$$

The Voigt components T_α form a Voigt matrix:

$$\begin{pmatrix} T_1 & T_6 & T_5 \\ & T_2 & T_4 \\ & & T_3 \end{pmatrix}.$$

The terms of the leading diagonal correspond to principal normal constraints and the non-diagonal terms to shears (see Section 1.3.2).

1.1.4.10.3. *Reduction of the number of independent components of third-rank polar tensors due to the symmetry of the strain and stress tensors*

Equation (1.1.4.5) can be written

$$P_i = \sum_j d_{ijj}T_{jj} + \sum_{j\neq k}(d_{ijk} + d_{ikj})T_{jk}.$$

The sums $(d_{ijk} + d_{ikj})$ for $j \neq k$ have a definite physical meaning, but it is impossible to devise an experiment that permits d_{ijk} and d_{ikj} to be measured separately. It is therefore usual to set them equal:

$$d_{ijk} = d_{ikj}. \qquad (1.1.4.7)$$

It was seen in Section 1.1.4.8.1 that the components of a third-rank tensor can be represented as a 9×3 matrix which can be subdivided into three 3×3 submatrices:

$$(\quad \mathbf{1} \quad | \quad \mathbf{2} \quad | \quad \mathbf{3} \quad).$$

Relation (1.1.4.7) shows that submatrices **1** and **2** are identical. One puts, introducing a two-index notation,

$$\left.\begin{array}{ll} d_{ijj} = d_{i\alpha} & (\alpha = 1, 2, 3) \\ d_{ijk} + d_{ikj}\ (j \neq k) = d_{i\alpha} & (\alpha = 4, 5, 6). \end{array}\right\}$$

Relation (1.1.4.7) becomes

$$P_i = d_{i\alpha}T_\alpha.$$

The coefficients $d_{i\alpha}$ may be written as a 3×6 matrix:

$$\begin{pmatrix} 11 & 12 & 13 & 14 & 15 & 16 \\ 21 & 22 & 23 & 24 & 25 & 26 \\ 31 & 32 & 33 & 34 & 35 & 36 \end{pmatrix}.$$

This matrix is constituted by two 3×3 submatrices. The left-hand one is identical to the submatrix **1**, and the right-hand one is equal to the sum of the two submatrices **2** and **3**:

$$(\quad \mathbf{1} \quad | \quad \mathbf{2 + 3} \quad).$$

The inverse piezoelectric effect expresses the strain in a crystal submitted to an applied electric field:

$$S_{ij} = d_{ijk}E_k,$$

where the matrix associated with the coefficients d_{ijk} is a 9×3 matrix which is the transpose of that of the coefficients used in equation (1.1.4.5), as shown in Section 1.1.1.4.

The components of the Voigt strain matrix S_α are then given by

$$\left.\begin{array}{ll} S_\alpha = d_{iik}E_k & (\alpha = 1, 2, 3) \\ S_\alpha = S_{ij} + S_{ji} = (d_{ijk} + d_{jik})E_k & (\alpha = 4, 5, 6). \end{array}\right\}$$

This relation can be written simply as

$$S_\alpha = d_{\alpha k}E_k,$$

where the matrix of the coefficients $d_{\alpha k}$ is a 6×3 matrix which is the transpose of the $d_{i\alpha}$ matrix.

There is another set of piezoelectric constants (see Section 1.1.5) which relates the stress, T_{ij}, and the electric field, E_k, which are both intensive parameters:

$$T_{ij} = e_{ijk}E_k, \qquad (1.1.4.8)$$

where a new piezoelectric tensor is introduced, e_{ijk}. Its components can be represented as a 3×9 matrix:

$$\begin{pmatrix} \mathbf{1} \\ \overline{\mathbf{2}} \\ \overline{\mathbf{3}} \end{pmatrix}.$$

Both sides of relation (1.1.4.8) remain unchanged if the indices i and j are interchanged, on account of the symmetry of the stress tensor. This shows that

$$e_{ijk} = e_{jik}.$$

Submatrices **2** and **3** are equal. One introduces here a two-index notation through the relation $e_{\alpha k} = e_{ijk}$, and the $e_{\alpha k}$ matrix can be written

$$\left(\frac{\mathbf{1}}{\mathbf{2}+\mathbf{3}} \right).$$

The relation between the full and the reduced matrix is therefore different for the d_{ijk} and the e_{kij} tensors. This is due to the particular property of the strain Voigt matrix (1.1.4.6), and as a consequence the relations between nonzero components of the reduced matrices are different for certain point groups $(3, 32, 3m, \bar{6}, \bar{6}2m)$.

1.1.4.10.4. *Independent components of the matrix associated with a third-rank polar tensor according to the following point groups*

1.1.4.10.4.1. *Triclinic system*

(i) Group 1: all the components are independent. There are 18 components.
(ii) Group $\bar{1}$: all the components are equal to zero.

1.1.4.10.4.2. *Monoclinic system*

(i) Group 2: twofold axis parallel to Ox_2:

There are 8 independent components.
(ii) Group m:

There are 10 independent components.
(iii) Group $2/m$: all the components are equal to zero.

1.1.4.10.4.3. *Orthorhombic system*

(i) Group 222:

There are 3 independent components.

(ii) Group $mm2$:

There are 5 independent components.
(iii) Group mmm: all the components are equal to zero.

1.1.4.10.4.4. *Trigonal system*

(i) Group 3:

where the symbol $\ominus$ means that the corresponding component is equal to the opposite of that to which it is linked, $\odot$ means that the component is equal to twice minus the value of the component to which it is linked for d_{ijk} and to minus the value of the component to which it is linked for e_{ijk}. There are 6 independent components.
(ii) Group 32, twofold axis parallel to Ox_1:

with the same conventions. There are 4 independent components.
(iii) Group $3m$, mirror perpendicular to Ox_1:

with the same conventions. There are 4 independent components.
(iv) Groups $\bar{3}$ and $\bar{3}m$: all the components are equal to zero.

1.1.4.10.4.5. *Tetragonal, hexagonal and cylindrical systems*

(i) Groups 4, 6 and A_∞:

There are 4 independent components.
(ii) Groups 422, 622 and $A_\infty \infty A_2$:

There is 1 independent component.
(iii) Groups $4mm$, $6mm$ and $A_\infty \infty M$:

There are 3 independent components.

(iv) Groups $4/m$, $6/m$ and $(A_\infty/M)C$: all the components are equal to zero.
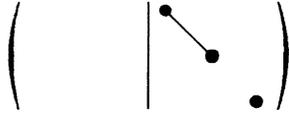
(v) Group $\bar{4}$:
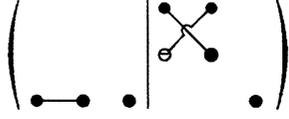
There are 4 independent components.
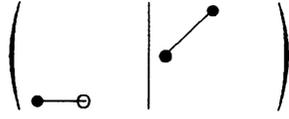
(vi) Group $\bar{6} = 3/m$:
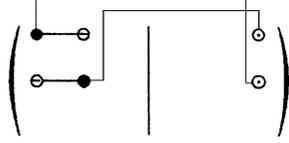
with the same conventions as for group 3. There are 2 independent components.

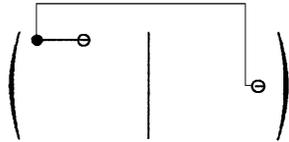(vii) Group $\bar{4}2m$ – twofold axis parallel to Ox_1:

There are 2 independent components.

(viii) Group $\bar{4}2m$ – mirror perpendicular to Ox_1 (twofold axis at 45°):

The number of independent components is of course the same.

(ix) Group $\bar{6}2/m$:

with the same conventions as for group 3. There is 1 independent component.

(x) Groups $4/mm$, $6/mm$ and $(A_\infty/M)\infty(A_2/M)C$: all the components are equal to zero.

1.1.4.10.4.6. *Cubic and spherical systems*

(i) Groups 23 and $\bar{4}3m$:
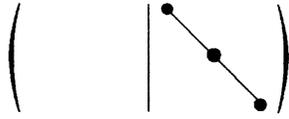
There is 1 independent component.

(ii) Groups 432 and ∞A_∞: it was seen in Section 1.1.4.8.6 that we have in this case

$$d_{123} = -d_{132}.$$

It follows that $d_{14} = 0$, all the components are equal to zero.

(iii) Groups $m\bar{3}$, $m\bar{3}m$ and $\infty(A_\infty/M)C$: all the components are equal to zero.

1.1.4.10.5. *Reduction of the number of independent components of fourth-rank polar tensors due to the symmetry of the strain and stress tensors*

Let us consider five examples of fourth-rank tensors:

(i) *Elastic compliances*, s_{ijkl}, relating the resulting strain tensor S_{ij} to an applied stress T_{ij} (see Section 1.3.3.2):

$$S_{ij} = s_{ijkl}T_{kl}, \tag{1.1.4.9}$$

where the compliances s_{ijkl} are the components of a tensor of rank 4.

(ii) *Elastic stiffnesses*, c_{ijkl} (see Section 1.3.3.2):

$$T_{ij} = c_{ijkl}S_{kl}.$$

(iii) *Piezo-optic coefficients*, π_{ijkl}, relating the variation $\Delta\eta_{ij}$ of the dielectric impermeability to an applied stress T_{kl} (*photoelastic effect* – see Section 1.6.7):

$$\Delta\eta_{ij} = \pi_{ijkl}T_{kl}.$$

(iv) *Elasto-optic coefficients*, p_{ijkl}, relating the variation $\Delta\eta_{ij}$ of the dielectric impermeability to the strain S_{kl}:

$$\Delta\eta_{ij} = p_{ijkl}S_{kl}.$$

(v) *Electrostriction coefficients*, Q_{ijkl}, which appear in equation (1.1.4.4):

$$S_{ij} = Q_{ijkl}E_kE_l, \tag{1.1.4.10}$$

where only the second-order terms are considered.

In each of the equations from (1.1.4.9) to (1.1.4.10), the contracted product of a fourth-rank tensor by a symmetric second-rank tensor is equal to a symmetric second-rank tensor. As in the case of the third-rank tensors, this results in a reduction of the number of independent components, but because of the properties of the strain Voigt matrix, and because two of the tensors are endowed with intrinsic symmetry (the elastic tensors), the reduction is different for each of the five tensors. The above relations can be written in matrix form:

1		1	2	3		1
2	=	4	5	6	×	2
3		7	8	9		3

where the second-rank tensors are represented by 1×9 column matrices, which can each be subdivided into three 1×3 submatrices and the 9×9 matrix associated with the fourth-rank tensors is subdivided into nine 3×3 submatrices, as shown in Section 1.1.4.9.1. The symmetry of the second-rank tensors means that submatrices **2** and **3** which are associated with them are equal.

Let us first consider the reduction of the tensor of elastic compliances. As in the case of the piezoelectric tensor, equation (1.1.4.9) can be written

$$S_{ij} = \sum_l s_{ijll}T_{ll} + \sum_{k\neq l}(s_{ijkl} + s_{ijlk})T_{kl}. \tag{1.1.4.11}$$

The sums $(s_{ijkl} + s_{ijlk})$ for $k \neq l$ have a definite physical meaning, but it is impossible to devise an experiment permitting s_{ijkl} and s_{ijlk} to be measured separately. It is therefore usual to set them equal in order to avoid an unnecessary constant:

$$s_{ijkl} = s_{ijlk}.$$

Furthermore, the left-hand term of (1.1.4.11) remains unchanged if we interchange the indices i and j. The terms on the right-hand side therefore also remain unchanged, whatever the value of T_{ll} or T_{kl}. It follows that

$$s_{ijll} = s_{jill}$$
$$s_{ijkl} = s_{ijlk} = s_{jikl} = s_{jilk}.$$

Similar relations hold for c_{ijkl}, Q_{ijkl}, p_{ijkl} and π_{ijkl}: the submatrices **2** and **3**, **4** and **7**, **5**, **6**, **8** and **9**, respectively, are equal.

Equation (1.4.1.11) can be rewritten, introducing the coefficients of the Voigt strain matrix:

$$S_\alpha = S_{ii} = \sum_l s_{iill} T_{ll} + \sum_{k \neq l} (s_{iikl} + s_{iilk}) T_{kl} \quad (\alpha = 1, 2, 3)$$

$$S_\alpha = S_{ij} + S_{ji} = \sum_l (s_{ijll} + s_{jill}) T_{ll}$$
$$+ \sum_{k \neq l} (s_{ijkl} + s_{ijlk} + s_{jikl} + s_{jilk}) T_{kl} \quad (\alpha = 4, 5, 6).$$

We shall now introduce a two-index notation for the elastic compliances, according to the following conventions:

$$\left.\begin{array}{llll} i = j; & k = l; & s_{\alpha\beta} = s_{iill} \\ i = j; & k \neq l; & s_{\alpha\beta} = s_{iikl} + s_{iilk} \\ i \neq j; & k = l; & s_{\alpha\beta} = s_{ijkk} + s_{jikk} \\ i \neq j; & k \neq l; & s_{\alpha\beta} = s_{ijkl} + s_{jikl} + s_{ijlk} + s_{jilk}. \end{array}\right\} \quad (1.1.4.12)$$

We have thus associated with the fourth-rank tensor a square 6×6 matrix with 36 coefficients:

β / α	1	2	3	4	5	6
1	11	12	13	14	15	16
2	21	22	23	24	25	26
3	31	32	33	34	35	36
4	41	42	43	44	45	46
5	51	52	53	54	55	56
6	61	62	63	64	65	66

One can translate relation (1.1.4.12) using the 9×9 matrix representing s_{ijkl} by adding term by term the coefficients of submatrices **2** and **3**, **4** and **7** and **5**, **6**, **8** and **9**, respectively:

$$\left(\begin{array}{c} 1 \\ \hline 2+3 \end{array}\right) = \left(\begin{array}{c|c} 1 & 2 \\ \hline 4+7 & \begin{array}{c} 5+6 \\ +8+9 \end{array} \end{array}\right) \times \left(\begin{array}{c} 1 \\ \hline 2+3 \end{array}\right)$$

Using the two-index notation, equation (1.1.4.9) becomes

$$S_\alpha = s_{\alpha\beta} T_\beta. \quad (1.1.4.13)$$

A similar development can be applied to the other fourth-rank tensors π_{ijkl}, which will be replaced by 6×6 matrices with 36 coefficients, according to the following rules.

(i) *Elastic stiffnesses*, c_{ijkl} and *elasto-optic coefficients*, p_{ijkl}:

$$\left(\begin{array}{c} 1 \\ \hline 2 \end{array}\right) = \left(\begin{array}{c|c} 1 & 2 \\ \hline 4 & 5 \end{array}\right) \times \left(\begin{array}{c} 1 \\ \hline 2 \end{array}\right)$$

where

$$c_{\alpha\beta} = c_{ijkl}$$
$$p_{\alpha\beta} = p_{ijkl}.$$

(ii) *Piezo-optic coefficients*, π_{ijkl}:

$$\left(\begin{array}{c} 1 \\ \hline 2 \end{array}\right) = \left(\begin{array}{c|c} 1 & 2+3 \\ \hline 4 & 5+6 \end{array}\right) \times \left(\begin{array}{c} 1 \\ \hline 2 \end{array}\right)$$

where

$$\left.\begin{array}{llll} i = j; & k = l; & \pi_{\alpha\beta} = \pi_{iill} \\ i = j; & k \neq l; & \pi_{\alpha\beta} = \pi_{iikl} + \pi_{iilk} \\ i \neq j; & k = l; & \pi_{\alpha\beta} = \pi_{ijkk} = \pi_{jikk} \\ i \neq j; & k \neq l; & \pi_{\alpha\beta} = \pi_{ijkl} + \pi_{jikl} = \pi_{ijlk} + \pi_{jilk}. \end{array}\right\}$$

(iii) *Electrostriction coefficients*, Q_{ijkl}: same relation as for the elastic compliances.
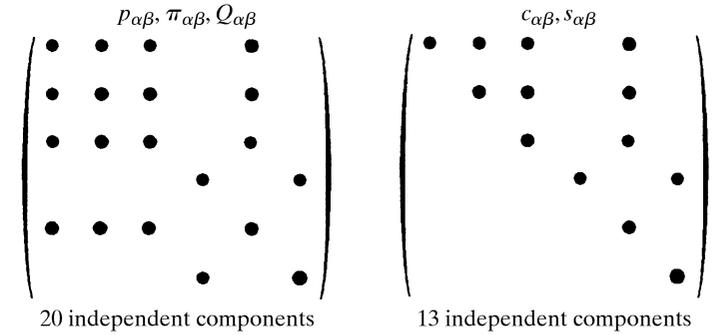
1.1.4.10.6. *Independent components of the matrix associated with a fourth-rank tensor according to the following point groups*

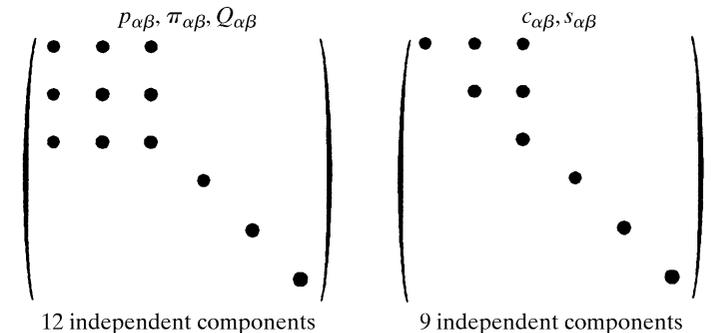1.1.4.10.6.1. *Triclinic system, groups* $\bar{1}$, 1

$p_{\alpha\beta}, \pi_{\alpha\beta}, Q_{\alpha\beta}$ — 36 independent components

$c_{\alpha\beta}, s_{\alpha\beta}$ — 21 independent components
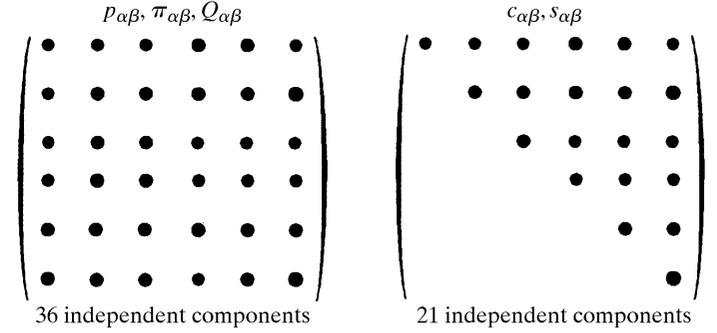
1.1.4.10.6.2. *Monoclinic system*

Groups $2/m$, 2, m, twofold axis parallel to Ox_2:

$p_{\alpha\beta}, \pi_{\alpha\beta}, Q_{\alpha\beta}$ — 20 independent components

$c_{\alpha\beta}, s_{\alpha\beta}$ — 13 independent components

1.1.4.10.6.3. *Orthorhombic system*

Groups mmm, $2mm$, 222:

$p_{\alpha\beta}, \pi_{\alpha\beta}, Q_{\alpha\beta}$ — 12 independent components

$c_{\alpha\beta}, s_{\alpha\beta}$ — 9 independent components

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1.1.4.10.6.4. *Trigonal system*

(i) Groups 3, $\bar{3}$:

$p_{\alpha\beta}$

12 independent components

$\pi_{\alpha\beta}$

12 independent components

$Q_{\alpha\beta}$

12 independent components

$c_{\alpha\beta}$

7 independent components
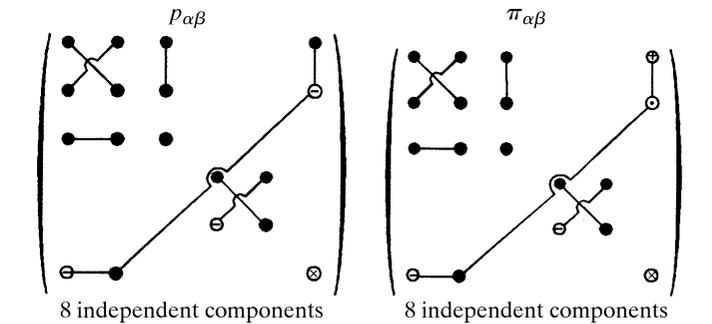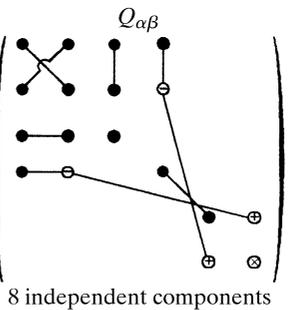

$s_{\alpha\beta}$

7 independent components

where $\ominus$ is a component numerically equal but opposite in sign to the heavy dot component to which it is linked; $\oplus$ is a component equal to twice the heavy dot component to which it is linked; $\odot$ is a component equal to minus twice the heavy dot component to which it is linked; $\otimes$ is equal to $1/2(p_{11} - p_{12})$, $(\pi_{11} - \pi_{12})$, $2(Q_{11} - Q_{12})$, $1/2(c_{11} - c_{12})$ and $2(s_{11} - s_{12})$, respectively.
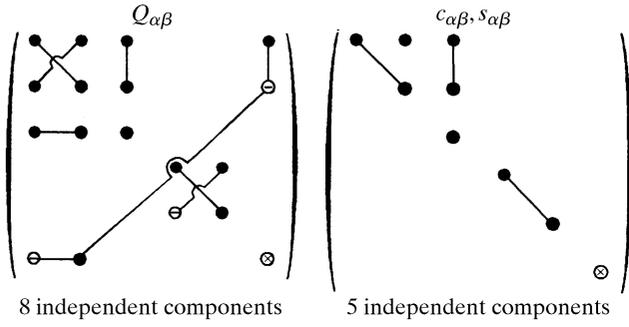
(ii) Groups 32, 3m, $\bar{3}m$:

$p_{\alpha\beta}$

8 independent components

$\pi_{\alpha\beta}$

8 independent components

$Q_{\alpha\beta}$

8 independent components

$c_{\alpha\beta}$

6 independent components

$s_{\alpha\beta}$

6 independent components

with the same conventions.

1.1.4.10.6.5. *Tetragonal system*

(i) Groups 4, $\bar{4}$ and $4/m$:

$p_{\alpha\beta}, \pi_{\alpha\beta}, Q_{\alpha\beta}$

10 independent components

$c_{\alpha\beta}, s_{\alpha\beta}$

7 independent components
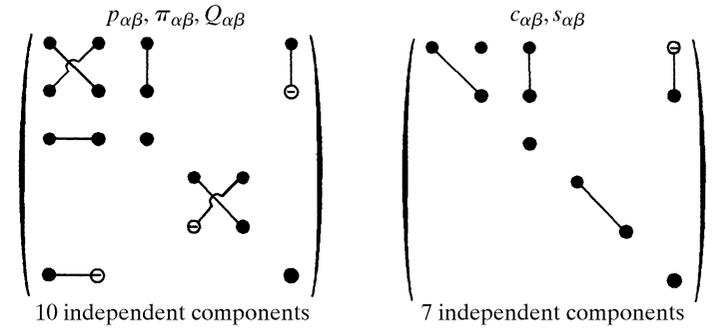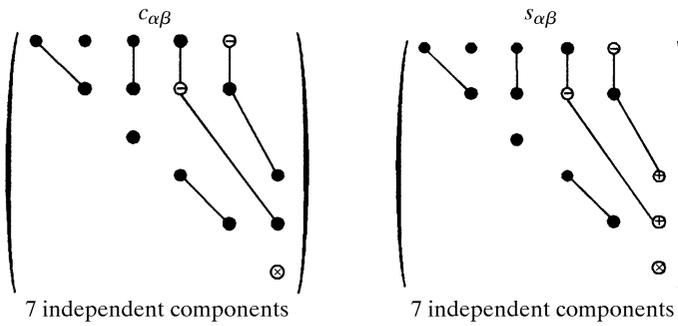
(ii) Groups 422, 4mm, $\bar{4}2m$ and $4/mm$:

$p_{\alpha\beta}, \pi_{\alpha\beta}, Q_{\alpha\beta}$

7 independent components

$c_{\alpha\beta}, s_{\alpha\beta}$

6 independent components
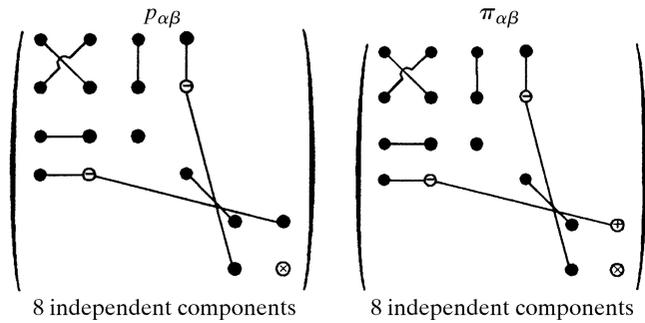
1.1.4.10.6.6. *Hexagonal system*

(i) Groups 6, $\bar{6}$ and $6/m$:

$p_{\alpha\beta}$

8 independent components

$\pi_{\alpha\beta}$

8 independent components

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$Q_{\alpha\beta}$

$c_{\alpha\beta}, s_{\alpha\beta}$

8 independent components   5 independent components

1.1.4.10.6.8. *Spherical system*

For all tensors

$p_{\alpha\beta}, \pi_{\alpha\beta}, Q_{\alpha\beta}, c_{\alpha\beta}, s_{\alpha\beta}$

2 independent components
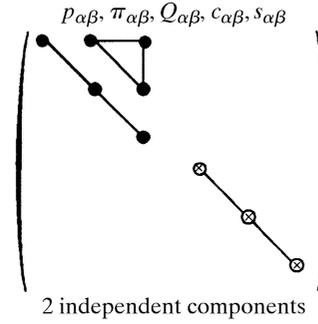
(ii) Groups 622, 6*mm*, $\bar{6}2m$ and 6/*mm*:

$p_{\alpha\beta}, \pi_{\alpha\beta}, Q_{\alpha\beta}$

$c_{\alpha\beta}, s_{\alpha\beta}$

6 independent components   5 independent components
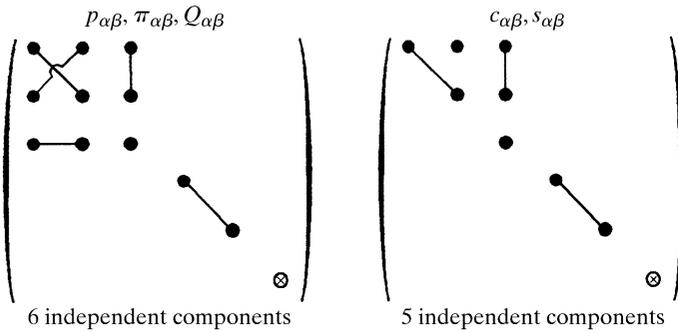
1.1.4.10.7. *Reduction of the number of independent components of axial tensors of rank 2*

It was shown in Section 1.1.4.5.3.2 that axial tensors of rank 2 are actually tensors of rank 3 antisymmetric with respect to two indices. The matrix of independent components of a tensor such that

$$g_{ijk} = -g_{jik}$$

is given by

$$\begin{pmatrix} & 122 & 133 & 123 & 131 & 132 & & 121 \\ -121 & & 223 & & 231 & -122 & 232 & -123 \\ -131 & -232 & & -233 & & -132 & & -133 & -231 \end{pmatrix}.$$

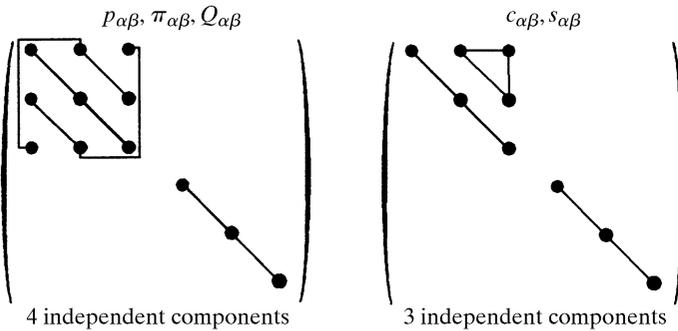The second-rank axial tensor g_{kl} associated with this tensor is defined by

$$g_{kl} = \tfrac{1}{2}\varepsilon_{ijk}g_{ijl}.$$

For instance, the piezomagnetic coefficients that give the magnetic moment M_i due to an applied stress T_α are the components of a second-rank axial tensor, $\Lambda_{i\alpha}$ (see Section 1.5.7.1):

$$M_i = \Lambda_{i\alpha}T_\alpha.$$

1.1.4.10.6.7. *Cubic system*
(i) Groups 23 and 3*m*:

$p_{\alpha\beta}, \pi_{\alpha\beta}, Q_{\alpha\beta}$

$c_{\alpha\beta}, s_{\alpha\beta}$

4 independent components   3 independent components

1.1.4.10.7.1. *Independent components according to the following point groups*
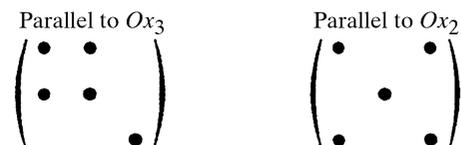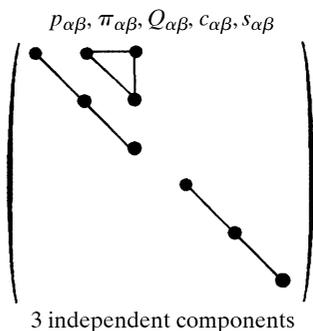
(i) *Triclinic system*
(*a*) Group 1:

(*b*) Group $\bar{1}$: all components are equal to zero.
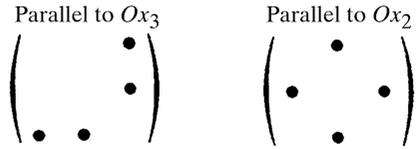(ii) *Monoclinic system*
(*a*) Group 2:

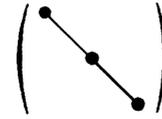(ii) Groups 432, $\bar{4}3m$ and $m\bar{3}m$:

$p_{\alpha\beta}, \pi_{\alpha\beta}, Q_{\alpha\beta}, c_{\alpha\beta}, s_{\alpha\beta}$

3 independent components

Parallel to Ox_3 Parallel to Ox_2

(*b*) Group *m*:

Parallel to Ox_3 Parallel to Ox_2

(*c*) Group 2/*m*: all components are equal to zero.

(iii) *Orthorhombic system*
(*a*) Group 222:

(*b*) Group *mm*2:

(*c*) Group *mmm*: all components are equal to zero.

(iv) *Trigonal, tetragonal, hexagonal and cylindrical systems*
(*a*) Groups 3, 4, 6 and A_∞:

(*b*) Groups 32, 42, 62 and $A_\infty \infty A_2$:
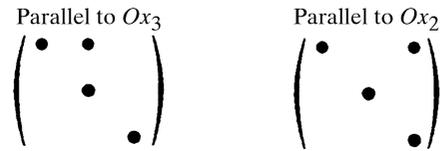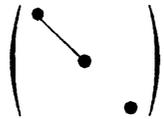
(*c*) Groups 3*m*, 4*m*, 6*m* and $A_\infty \infty M$:
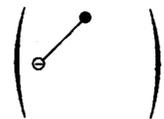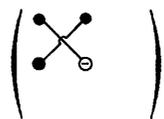
(*d*) Group $\bar{4}$:

(*e*) Group $\bar{4}2m$:
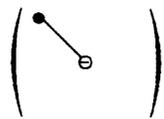
(*f*) Groups $\bar{3}$, 4/*m*, $\bar{6}2m$, $\bar{3}m$, 4/*mm* and 6/*mm*: all components are equal to zero.

(v) *Cubic and spherical systems*
(*a*) Groups 23, 432 and ∞A_∞:

The axial tensor is reduced to a pseudoscalar.
(*b*) Groups $m\bar{3}$, $\bar{4}3m$, $m\bar{3}m$ and $\infty(A_\infty/M)C$: all components are equal to zero.

1.1.4.10.7.2. *Independent components of symmetric axial tensors according to the following point groups*

Some axial tensors are also symmetric. For instance, the optical rotatory power of a gyrotropic crystal in a given direction of direction cosines $\alpha_1, \alpha_2, \alpha_3$ is proportional to a quantity G defined by (see Section 1.6.5.4)
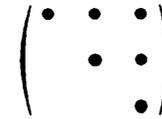
$$G = g_{ij}\alpha_i\alpha_j,$$

where the gyration tensor g_{ij} is an axial tensor. This expression shows that only the symmetric part of g_{ij} is relevant. This leads to a further reduction of the number of independent components:
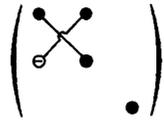(i) *Triclinic system*
(*a*) Group 1:

(*b*) Group $\bar{1}$: all components are equal to zero.
(ii) *Monoclinic system*
(*a*) Group 2:

Parallel to Ox_3 Parallel to Ox_2

(*b*) Group *m*:

Parallel to Ox_3 Parallel to Ox_2

(*c*) Group 2/*m*: all components are equal to zero.
(iii) *Orthorhombic system*
(*a*) Group 222:

(*b*) Group *mm*2:

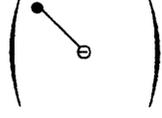(*c*) Group *mmm*: all components are equal to zero.

(iv) *Trigonal, tetragonal and hexagonal systems*
(*a*) Groups 3, 32, 4, 42, 6, 62:
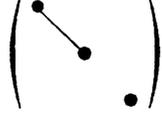
(*b*) Group $\bar{4}$:
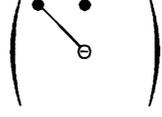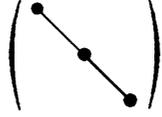
(*c*) Group $\bar{4}2m$:

(*d*) Groups $\bar{3}, 3m, \bar{3}m, 4/m, 4mm, 4/mm, \bar{6}, \bar{6}2m$ and $6/mm$: all components are equal to zero.
(v) *Cubic and spherical systems*
(*a*) Groups 23, 432 and $A_\infty \infty A_2$:

(*b*) Groups $m\bar{3}, \bar{4}3m, m\bar{3}m$ and $\infty(A_\infty/M)C$: all components are equal to zero.

In practice, gyrotropic crystals are only found among the enantiomorphic groups: 1, 2, 222, 3, 32, 4, 422, 6, 622, 23, 432. Pasteur (1848*a,b*) was the first to establish the distinction between 'molecular dissymmetry' and 'crystalline dissymmetry'.

1.1.5. Thermodynamic functions and physical property tensors

[The reader may also consult Mason (1966), Nye (1985) or Sirotin & Shaskol'skaya (1982).]

1.1.5.1. *Isothermal study*

The energy of a system is the sum of all the forms of energy: thermal, mechanical, electrical *etc.* Let us consider a system whose only variables are these three. For a small variation of the associated extensive parameters, the variation of the internal energy is

$$d\mathcal{U} = E_n \, dD_n + T_{kl} \, dS_{kl} + \Theta \, d\sigma,$$

where Θ is the temperature and σ is the entropy; there is summation over all dummy indices; an orthonormal frame is assumed and variance is not apparent. The mechanical energy of deformation is given by $T_{kl} \, dS_{kl}$ (see Section 1.3.2.8). Let us consider the Gibbs free-energy function $\mathcal{G}$ defined by

$$\mathcal{G} = \mathcal{U} - E_n D_n - T_{kl}S_{kl} - \Theta\sigma.$$

Differentiation of $\mathcal{G}$ gives

$$d\mathcal{G} = -D_n \, dE_n - S_{kl} \, dT_{kl} - \sigma \, d\Theta.$$

The extensive parameters are therefore partial derivatives of the free energy:

$$S_{kl} = -\frac{\partial \mathcal{G}}{\partial T_{kl}}; \quad D_n = -\frac{\partial \mathcal{G}}{\partial E_n}; \quad \sigma = -\frac{\partial \mathcal{G}}{\partial \Theta}.$$

Each of these quantities may be expanded by performing a further differentiation in terms of the intensive parameters, T_{kl}, E_n and Θ. We have, to the first order,

$$dS_{kl} = \left[\frac{\partial S_{kl}}{\partial T_{ij}}\right]_{E,\Theta} dT_{ij} + \left[\frac{\partial S_{kl}}{\partial E_n}\right]_{T,\Theta} dE_n + \left[\frac{\partial S_{kl}}{\partial \Theta}\right]_{E,T} \delta\Theta$$

$$dD_n = \left[\frac{\partial D_n}{\partial T_{kl}}\right]_{E,\Theta} dT_{kl} + \left[\frac{\partial D_n}{\partial E_m}\right]_{T,\Theta} dE_m + \left[\frac{\partial D_n}{\partial \Theta}\right]_{E,T} \delta\Theta$$

$$d\sigma = \left[\frac{\partial \sigma}{\partial T_{ij}}\right]_{E,\Theta} dT_{ij} + \left[\frac{\partial \sigma}{\partial E_m}\right]_{T,\Theta} dE_m + \left[\frac{\partial \sigma}{\partial \Theta}\right]_{E,T} \delta\Theta.$$

To a first approximation, the partial derivatives may be considered as constants, and the above relations may be integrated:

$$\left.\begin{aligned}
S_{kl} &= \left(s_{klij}\right)^{E,\Theta} T_{ij} &+ (d_{kln})^{T,\Theta} E_n &+ (\alpha_{kl})^{E,T} \delta\Theta \\
D_n &= (d_{nkl})^{E,\Theta} T_{kl} &+ (\varepsilon_{nm})^{T,\Theta} E_m &+ (p_n)^{E,T} \delta\Theta \\
\delta\sigma &= (\alpha_{ij})^{E} T_{ij} &+ (p_m)^{T} E_m &+ (\rho C^{E,T}/\Theta)\delta\Theta.
\end{aligned}\right\}$$

$$(1.1.5.1)$$

This set of equations is the equivalent of relation (1.1.1.6) of Section 1.1.1.3, which gives the coefficients of the matrix of physical properties. These coefficients are:

(i) For the principal properties: $\left(s_{klij}\right)^{E,\Theta}$: elastic compliances at constant temperature and field; $(\varepsilon_{nm})^{T,\Theta}$: dielectric constant at constant temperatures and stress; $\rho C^{T,E}$: heat capacity per unit volume at constant stress and field (ρ is the specific mass and $C^{T,E}$ is the specific heat at constant stress and field).

(ii) For the other properties: $(d_{kln})^{T,\Theta}$ and $(d_{nkl})^{E,\Theta}$ are the components of the piezoelectric effect and of the converse effect. They are represented by 3×9 and 9×3 matrices, respectively. One may notice that

$$d_{kln} = \frac{\partial S_{kl}}{\partial E_n} = -\frac{\partial^2 \mathcal{G}}{\partial E_n \partial T_{kl}} = -\frac{\partial^2 \mathcal{G}}{\partial T_{kl} \partial E_n} = \frac{\partial D_n}{\partial T_{kl}} = d_{nkl},$$

which shows again that the components of two properties that are symmetric with respect to the leading diagonal of the matrix of physical properties are equal (Section 1.1.1.4) and that the corresponding matrices are transpose to one another.

In a similar way,
(*a*) the matrices $(\alpha_{kl})^{E,T}$ of the thermal expansion and $(\alpha_{ij})^{E}$ of the piezocalorific effect are transpose to one another;
(*b*) the components $(p_n)^{T}$ of the pyroelectric and of the electrocalorific effects are equal.

Remark. The piezoelectric effect, namely the existence of an electric polarization **P** under an applied stress, is always measured at zero applied electric field and at constant temperature. The second equation of (1.1.5.1) becomes under these circumstances

$$P_n = D_n = (d_{nkl})^{\Theta} T_{kl}.$$

Remark. Equations (1.1.5.1) are, as has been said, first-order approximations because we have assumed the partial derivatives to be constants. Actually, this approximation is not correct, and in many cases it is necessary to take into account the higher-order terms as, for instance, in:
(*a*) nonlinear elasticity (see Sections 1.3.6 and 1.3.7);
(*b*) electrostriction;
(*c*) nonlinear optics (see Chapter 1.7);
(*d*) electro-optic and piezo-optic effects (see Sections 1.6.6 and 1.6.7).

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1.1.5.2. *Other forms of the piezoelectric constants*

We use here another Gibbs function, the electric Gibbs function, $\mathcal{G}_2$, defined by

$$\mathcal{G}_2 = \mathcal{U} - E_n D_n - \Theta \sigma.$$

Differentiation of $\mathcal{G}$ gives

$$d\mathcal{G}_2 = -D_n \, dE_n + T_{ij} \, dS_{ij} - \sigma \, d\Theta.$$

It follows that

$$T_{ij} = \frac{\partial \mathcal{G}_2}{\partial S_{ij}}; \quad D_n = -\frac{\partial \mathcal{G}_2}{\partial E_n}; \quad \sigma = -\frac{\partial \mathcal{G}_2}{\partial \Theta}$$

and a set of relations analogous to (1.1.5.1):

$$\left. \begin{array}{llll} T_{ij} = (c_{ijkl})^{E,\Theta} S_{kl} & - (e_{ijn})^{S,\Theta} E_n & - (\lambda_{ij})^{E,S} \, \delta\Theta \\ D_n = (e_{nij})^{E,\Theta} S_{ij} & + (\varepsilon_{nm})^{S,\Theta} E_m & + (p_n)^S \, \delta\Theta \\ \delta\sigma = (\lambda_{ij})^E S_{ij} & + (p_n)^S E_n & + \rho C^{E,S} \, \delta\Theta/\Theta, \end{array} \right\} \quad (1.1.5.2)$$

where the components $(c_{ijkl})^{E,\Theta}$ are the isothermal elastic stiffnesses at constant field and constant temperature,

$$e_{ijn} = -\frac{\partial T_{ij}}{\partial E_n} = -\frac{\partial^2 \mathcal{G}_2}{\partial E_n \partial S_{ij}} = -\frac{\partial^2 \mathcal{G}_2}{\partial S_{ij} \partial E_n} = \frac{\partial D_n}{\partial S_{ij}} = e_{nij}$$

are the piezoelectric stress coefficients at constant strain and constant temperature,

$$\lambda_{ij} = -\frac{\partial T_{ij}}{\partial \Theta} = -\frac{\partial^2 \mathcal{G}_2}{\partial \Theta \partial S_{ij}} = -\frac{\partial^2 \mathcal{G}_2}{\partial S_{ij} \partial \Theta} = \frac{\partial \delta\sigma}{\partial S_{ij}}$$

are the temperature-stress constants and

$$p_n = \frac{\partial D_n}{\partial \Theta} = -\frac{\partial^2 \mathcal{G}_2}{\partial \Theta \partial E_n} = -\frac{\partial^2 \mathcal{G}_2}{\partial E_n \partial \Theta} = \frac{\partial \delta\sigma}{\partial D_n}$$

are the components of the pyroelectric effect at constant strain.

The relations between these coefficients and the usual coefficients d_{kln} are easily obtained:

(i) At constant temperature and strain: if one puts $\delta\Theta = 0$ and $S_{kl} = 0$ in the first equation of (1.1.5.1) and (1.1.5.2), one obtains, respectively,

$$0 = s_{klij} T_{ij} + d_{kln} E_n$$
$$T_{ij} = -e_{ijn} E_n,$$

from which it follows that

$$d_{kln} = s_{klij} e_{ijn}$$

at constant temperature and strain.

(ii) At constant temperature and stress: if one puts $\delta\Theta = 0$ and $T_{ij} = 0$, one obtains in a similar way

$$S_{kl} = d_{kln} E_n$$
$$0 = c_{ijkl} S_{kl} - e_{ijn} E_n,$$

from which it follows that

$$e_{ijn} = c_{ijkl} d_{kln}$$

at constant temperature and stress.

1.1.5.3. *Relation between the pyroelectric coefficients at constant stress and at constant strain*

By combining relations (1.1.5.1) and (1.1.5.2), it is possible to obtain relations between the pyroelectric coefficients at constant stress, p_n^T, and the pyroelectric coefficients at constant strain, p_n^S, also called *real* pyroelectric coefficients, p_n^S. Let us put $T_{ij} = 0$ and $E_n = 0$ in the first equation of (1.1.5.1). For a given variation of temperature, $\delta\Theta$, the observed strain is

$$S_{kl} = \left[\alpha_{kl} \right]^{E,T} \delta\Theta.$$

From the second equations of (1.1.5.1) and (1.1.5.2), it follows that

$$D_n = p_n^T \delta\Theta$$
$$D_n = e_{nkl} S_{kl} + p_n \delta\Theta.$$

Substituting the expression S_{kl} and eliminating D_n, it follows that

$$p_n^T = e_{nkl} \left[\alpha_{kl} \right]^{E,T} + p_n^S. \quad (1.1.5.3)$$

This relation shows that part of the pyroelectric effect is actually due to the piezoelectric effect.

1.1.5.4. *Adiabatic study*

Piezoelectric resonators usually operate at a high frequency where there are no heat exchanges, and therefore in an adiabatic regime ($\Theta\delta\sigma = 0$). From the third equation of (1.1.5.1), we obtain a relation between the temperature variation, the applied stress and the electric field:

$$(\alpha_{ij})^E T_{ij} + (p_m)^T E_m + \frac{\rho C^{T,E}}{\Theta} \delta\Theta = 0.$$

If we substitute this relation in the two other relations of (1.1.5.1), we obtain two equivalent relations, but in the *adiabatic* regime:

$$S_{kl} = (s_{klij})^{E,\sigma} T_{ij} + (d_{klm})^{T,\sigma} E_m$$
$$D_n = (d_{nij})^{E,\sigma} T_{ij} + (\varepsilon_{nm})^{T,\sigma} E_m.$$

By comparing these expressions with (1.1.5.1), we obtain the following relations between the adiabatic and the isothermal coefficients:

$$(s_{ijkl})^{E,\sigma} = (s_{ijkl})^{E,\theta} - \frac{(\alpha_{ij})^E (\alpha_{kl})^E \Theta}{\rho C^{T,E}}$$

$$(d_{nij})^{E,\sigma} = (d_{nij})^{E,\theta} - \frac{(p_n)^T (\alpha_{kl})^E \Theta}{\rho C^{T,E}}$$

$$(\varepsilon_{mn})^{T,\sigma} = (\varepsilon_{mn})^{T,\theta} - \frac{(p_n)^T (p_m)^T \Theta}{\rho C^{T,E}}.$$

1.1.6. Glossary

$\mathbf{e}_i$	basis vectors in direct space (covariant)
$\mathbf{e}^i$	basis vectors in reciprocal space (contravariant)
x^i	components of a vector in direct space (contravariant)
x_i	components of a vector in reciprocal space (covariant)
g_{ij}	components of the metric tensor
$t_{i_1 \ldots i_p}^{j_1 \ldots j_q}$	components of a tensor of rank n, p times covariant and q times contravariant ($n = p + q$)
A^T	transpose of matrix A
$\otimes$	tensor product
$\bigwedge$	outer product
$\wedge$	vector product
∂_i	partial derivative with respect to x_i
δ_i	Kronecker symbol
ε_{ijk}	permutation tensor
V	volume

p	pressure
u_i	components of the displacement vector
S_{ij}	components of the strain tensor
S_α	components of the strain Voigt matrix
T_{ij}	components of the stress tensor
T_α	components of the stress Voigt matrix
s_{ijkl}	elastic compliances
$s_{\alpha\beta}$	reduced elastic compliances
$(s_{ijkl})^\sigma$	adiabatic elastic compliances
c_{ijkl}	elastic stiffnesses
$c_{\alpha\beta}$	reduced elastic stiffnesses
ν	Poisson's ratio
E	Young's modulus
Θ	temperature
σ	entropy
α_{ij}	thermal expansion
λ_{ij}	temperature-stress constant
$\mathcal{U}$	internal energy
$\mathcal{G}$	Gibbs free energy
$C^{E,T}$	specific heat at constant stress and applied electric field
$\mathbf{E}$	electric field
$\mathbf{D}$	electric displacement
$\mathbf{H}$	magnetic field
$\mathbf{B}$	magnetic induction
ε_o	permittivity of vacuum
ε	dielectric constant
ε_{ij}	dielectric tensor
$(\varepsilon_{ij})^\sigma$	adiabatic dielectric tensor
χ_e	dielectric susceptibility
η_{ij}	dielectric impermeability
p_i	pyroelectric tensor
d_{ijk}	piezoelectric tensor
$d_{i\alpha}$	reduced piezoelectric tensor
$d_{\alpha i}$	reduced inverse piezoelectric tensor
$(d_{ijk})^\sigma$	adiabatic piezoelectric tensor
e_{ijk}	piezoelectric tensor at constant strain
Q_{ijkl}	electrostriction tensor
$Q_{\alpha\beta}$	reduced electrostriction tensor
π_{ijkl}	piezo-optic tensor
$\pi_{\alpha\beta}$	reduced piezo-optic tensor
p_{ijkl}	elasto-optic tensor
$p_{\alpha\beta}$	reduced elasto-optic tensor
$R_{H\ ijk}$	Hall constant

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