

1. TENSORIAL ASPECTS OF PHYSICAL PROPERTIES

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

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

It is easy to check that

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

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

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

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:

$$x^i = A_j^i x^j.$$

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

$$A_j^i = \partial x^i / \partial x^j = \partial_j x^i.$$

It should be noted that the covariance has been increased.

1.1.3.8.2. Generalization

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

$$t_i^j = A_i^\alpha B_\beta^j t'_\alpha{}^\beta.$$

Differentiate with respect to x^k :

$$\begin{aligned} \frac{\partial t_i^j}{\partial x^k} &= \partial_k t_i^j = A_i^\alpha B_\beta^j \frac{\partial t'_\alpha{}^\beta}{\partial x'^\gamma} \frac{\partial x'^\gamma}{\partial x^k} \\ \partial_k t_i^j &= A_i^\alpha B_\beta^j A_k^\gamma \partial_\gamma t'_\alpha{}^\beta. \end{aligned}$$

It can be seen that the partial derivatives $\partial_k t_i^j$ 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_i^j . 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 $\mathbf{u}(\mathbf{r})$ be a vector function. Its development as a Taylor series is written

$$u^i(\mathbf{r} + d\mathbf{r}) = u^i(\mathbf{r}) + \frac{\partial u^i}{\partial x^j} dx^j + \frac{1}{2} \frac{\partial^2 u^i}{\partial x^j \partial x^k} dx^j dx^k + \dots \quad (1.1.3.5)$$

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

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

$$D^i = \varepsilon_j^i E^j + \chi_{jk}^i E^j E^k + \dots$$

(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), Sirotnin & Shaskol'skaya (1982), and Wooster (1973).

1.1. INTRODUCTION TO THE PROPERTIES OF TENSORS

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.

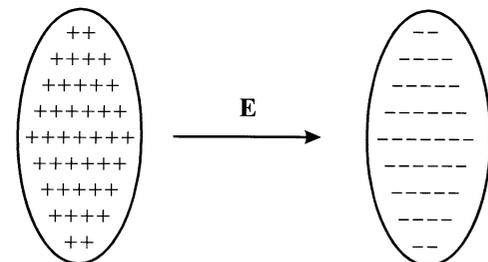


Fig. 1.1.4.1. Symmetry of an electric field.

1. TENSORIAL ASPECTS OF PHYSICAL PROPERTIES

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 piezoelectricity

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

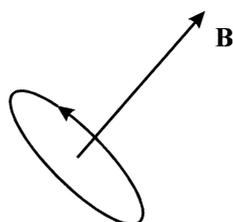


Fig. 1.1.4.2. Symmetry of magnetic induction.

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:

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

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 $32 = A_33A_2$. The above condition becomes

$$\frac{A_\infty \infty A_2}{M \infty M} C \cap A_33A_2 \leq A_\infty \infty M.$$

If the applied compression is parallel to the threefold axis, the intersection is identical to the symmetry of the crystal, A_33A_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. INTRODUCTION TO THE PROPERTIES OF TENSORS

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 dielectric 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. TENSORIAL ASPECTS OF PHYSICAL PROPERTIES

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 satisfies 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

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

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

$$t_k^l = \frac{1}{2}\varepsilon_{ijk}t^{ijl}$$

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

$$E_i = R_H \varepsilon_{ikl} j_k B_l,$$

where $R_H \varepsilon_{ikl}$ 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

$$R_H \varepsilon_{ikl} = -R_H \varepsilon_{kil},$$

which shows that $R_H \varepsilon_{ikl}$ 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

$$R_H \varepsilon_{123} = -R_H \varepsilon_{213}; \quad R_H \varepsilon_{132} = -R_H \varepsilon_{312}; \quad R_H \varepsilon_{312}; \quad R_H \varepsilon_{321}.$$

(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

$$c_{ijkl}(\omega, \mathbf{k}) = c_{ijkl}(\omega) + id_{ijklm}(\omega)k_m + \dots,$$

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), Sirotnin & 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

$$t_{\gamma\delta}^{\alpha\beta} = t_{kl}^{ij} A_i^\alpha A_j^\beta B_\gamma^k B_\delta^l.$$

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

1.1. INTRODUCTION TO THE PROPERTIES OF TENSORS

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

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

$$t_{\gamma\delta}^{\alpha\beta} = t_{\gamma\delta}^{\alpha\beta}$$

and, therefore,

$$t_{\gamma\delta}^{\alpha\beta} = t_{kl}^{ij} A_i^\alpha A_j^\beta B_\gamma^k B_\delta^l. \quad (1.1.4.1)$$

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

$$t_{kl}^{ij} = t_{kl}^{ij} A_i^\alpha A_j^\beta B_\gamma^k B_\delta^l \quad (1.1.4.2)$$

(without any summation).

If the product $A_i^\alpha A_j^\beta B_\gamma^k B_\delta^l$ (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 $t_{kl}^{ij} = 0$. 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*, $t^{ij\dots} = (-1)^{2p} t^{ij\dots}$. 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, $3m$
$4/m$	4, 4
$4/m\bar{m}$	422, $4mm$
$6/m$	6, 6
$6/m\bar{m}$	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*, $t^{ij\dots} = (-1)^{2p+1} t^{ij\dots}$. 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^α by their expression, (1.1.4.2) becomes, for a proper rotation,

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

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 $t^{jk\dots}$ 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 :

$$T = BTB^T,$$

1. TENSORIAL ASPECTS OF PHYSICAL PROPERTIES

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 (1952a,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

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

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

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

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):

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

where the sign \bullet represents a nonzero component.

1.1.4.7.2. Monoclinic system

Groups $2m, 2, m$: 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

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

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

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

1.1.4.7.3. Orthorhombic system

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

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

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 $\bar{3}, 3; 4/m, \bar{4}, 4; 6/m, \bar{6}, 6; (A_\infty/M)C, A_\infty$

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

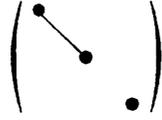
$$\begin{pmatrix} \bullet & \ominus & \bullet \\ \ominus & \bullet & \\ & & \bullet \end{pmatrix}$$

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. INTRODUCTION TO THE PROPERTIES OF TENSORS

1.1.4.7.4.2. Groups $\bar{3}m$, 32 , $3m$; $4/m\bar{m}$, 422 , $4mm$, $\bar{4}2m$; $6/m\bar{m}$, 622 , $6mm$, $62m$; $(A_\infty/M) \propto (A_2/M)C$, $A_\infty \propto A_2$

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



There are 2 independent components.

1.1.4.7.5. Cubic and spherical systems

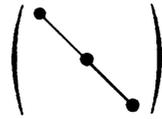
The cubic system is characterized by the presence of threefold axes along the $\langle 111 \rangle$ directions. The action of a threefold axis along $[111]$ on the components x_1, x_2, x_3 of a vector results in a permutation of these components, which become, respectively, x_2, x_3, x_1 and then x_3,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



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



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)



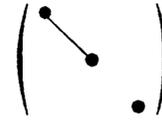
There are 4 independent components. The quadric is still any quadric, but one of its axes coincides with the twofold axis of the monoclinic lattice. Four parameters are required: the lengths of the axes and one angle.

1.1.4.7.6.3. Orthorhombic system



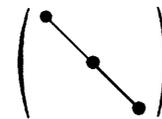
There are 3 independent components. The quadric is any quadric, the axes of which coincide with the crystallographic axes. Only three parameters are required.

1.1.4.7.6.4. Trigonal, tetragonal and hexagonal systems, isotropic groups



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



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.

1. TENSORIAL ASPECTS OF PHYSICAL PROPERTIES

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

$$\left(\begin{array}{ccc|ccc} \bullet & & & \bullet & \bullet & \\ & \bullet & & \bullet & & \\ & & \bullet & & & \bullet \end{array} \right)$$

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

$$\left(\begin{array}{ccc|ccc} \bullet & & & \bullet & \bullet & \bullet \\ & \bullet & & & & \\ & & \bullet & \bullet & \bullet & \bullet \end{array} \right)$$

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:

$$\left(\begin{array}{ccc|ccc} \bullet & \bullet & \bullet & \bullet & & \bullet \\ \bullet & \bullet & \bullet & & \bullet & \bullet \\ & & & \bullet & & \bullet \end{array} \right)$$

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

$$\left(\begin{array}{ccc|ccc} \bullet & \bullet & \bullet & \bullet & & \bullet \\ & \bullet & & & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & & \bullet \end{array} \right)$$

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.

$$\left(\begin{array}{ccc|ccc} & & & \bullet & & \\ & & & & \bullet & \\ & & & & & \bullet \end{array} \right)$$

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 :

$$\left(\begin{array}{ccc|ccc} & & & \bullet & & \\ & & & & \bullet & \\ & & & & & \bullet \end{array} \right)$$

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

$$\left(\begin{array}{ccc|ccc} \bullet & \ominus & & \bullet & \bullet & \ominus \\ \ominus & \bullet & & \bullet & \bullet & \ominus \\ \bullet & \bullet & \bullet & \bullet & \bullet & \ominus \end{array} \right)$$

There are 9 independent components.

1.1.4.8.4.2. Group 32 with a twofold axis parallel to Ox_1

$$\left(\begin{array}{ccc|ccc} \bullet & \ominus & & \bullet & & \ominus \\ & \bullet & & & \bullet & \ominus \\ & & \bullet & \bullet & \bullet & \ominus \end{array} \right)$$

There are 4 independent components.

1.1.4.8.4.3. Group $3m$ with a mirror normal to Ox_1

$$\left(\begin{array}{ccc|ccc} \bullet & \ominus & & \bullet & & \ominus \\ \ominus & \bullet & & \bullet & & \ominus \\ \bullet & \bullet & \bullet & \bullet & & \ominus \end{array} \right)$$

There are 4 independent components.

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

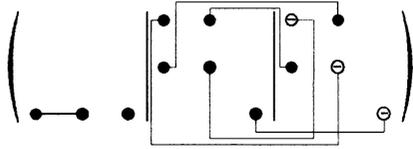
All the components are equal to zero.

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

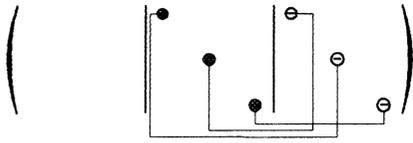
1.1. INTRODUCTION TO THE PROPERTIES OF TENSORS



There are 7 independent components.

1.1.4.8.5.2. Group 422

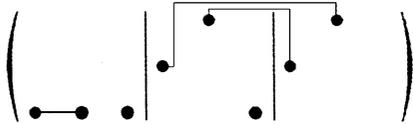
One combines the reductions for groups 4 and 222:



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

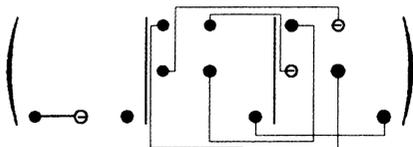
All the components are equal to zero.

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

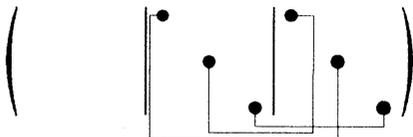


There are 6 independent components.

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

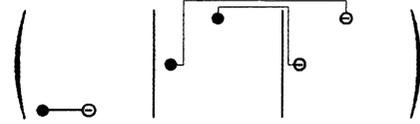
One combines either the reductions for groups $\bar{4}$ and 222, or the reductions for groups 4 and 2mm.

(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/m

All the components are equal to zero.

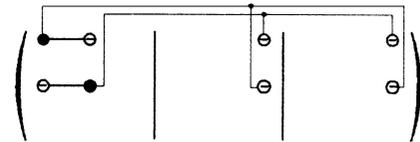
1.1.4.8.6. Hexagonal and cylindrical systems

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 $\bar{6} = 3/m$

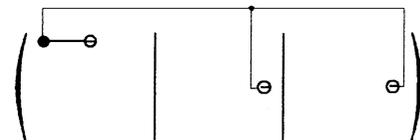
One combines the reductions for the groups corresponding to a threefold axis parallel to Ox_3 and to a mirror perpendicular to Ox_3 :



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.

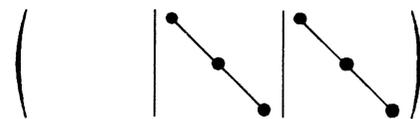
1.1.4.8.6.4. Groups 6/m, $(A_\infty/M)C$, 6/mm and $(A_\infty/M) \infty (A_2/M)C$

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 $[111]$:

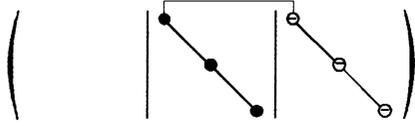


There are 2 independent components.

1. TENSORIAL ASPECTS OF PHYSICAL PROPERTIES

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

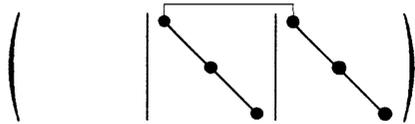
One combines the reductions corresponding to groups 422 and 23:



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.

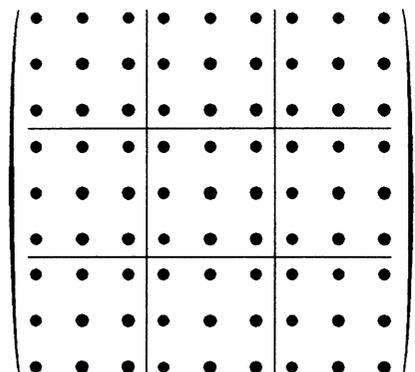
1.1.4.9. Reduction of the components of a tensor of rank 4

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:

ij	kl	11	22	33	23	31	12	32	13	21
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	

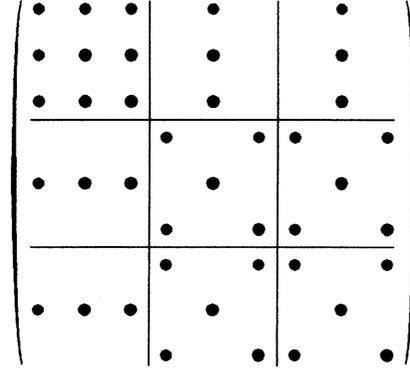
This matrix can be represented symbolically by



where the 9×9 matrix has been subdivided for clarity in to nine 3×3 submatrices.

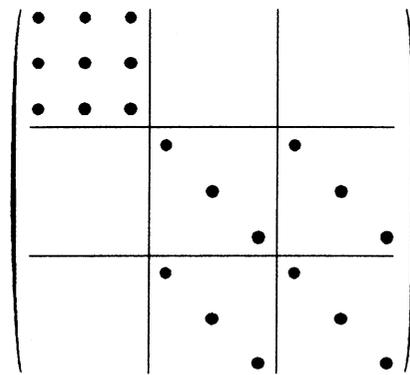
1.1.4.9.2. Monoclinic system (groups $2/m$, 2 , m)

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:

ij	kl	11	22	33	23	31	12	32	13	21
11	1111	1122	1133	1123	-2231	1112	1132	-2213	1121	
22	1122	1111	1133	-1123	2231	-1121	-1132	2213	-1121	
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	-1211	-1233	2213	1132	1221	2231	1123	1221	

with

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

There are 27 independent components.

1.1. INTRODUCTION TO THE PROPERTIES OF TENSORS

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

kl	11	22	33	23	31	12	32	13	21
ij									
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	11	22	33	23	31	12	32	13	21
ij									
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 $4/m\bar{m}2$, 422 , $4mm$, $\bar{4}2m$

kl	11	22	33	23	31	12	32	13	21
ij									
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	11	22	33	23	31	12	32	13	21
ij									
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

with

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

There are 19 independent components.

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

kl	11	22	33	23	31	12	32	13	21
ij									
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

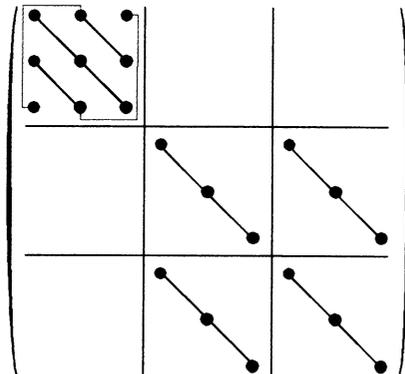
with

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

There are 11 independent components.

1.1.4.9.7. Cubic system

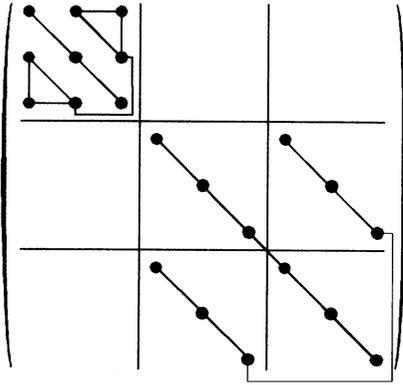
1.1.4.9.7.1. Groups 23 , $\bar{3}m$



There are 7 independent components.

1. TENSORIAL ASPECTS OF PHYSICAL PROPERTIES

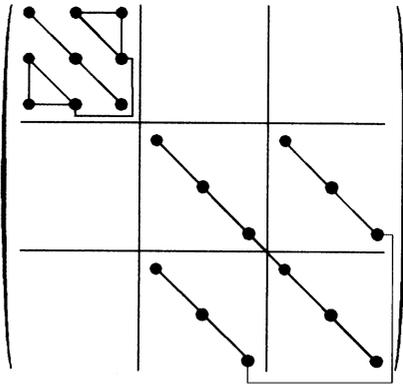
1.1.4.9.7.2. Groups $m\bar{3}m$, 432 , $\bar{4}3m$



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

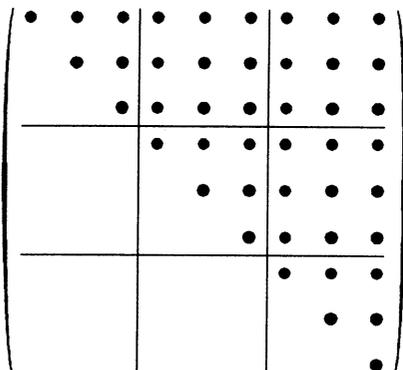
$$t_{1111} - t_{1122} = t_{1212} + t_{1221}.$$

There are 3 independent components. The tensor is symmetric.

1.1.4.9.9. Symmetric tensors of rank 4

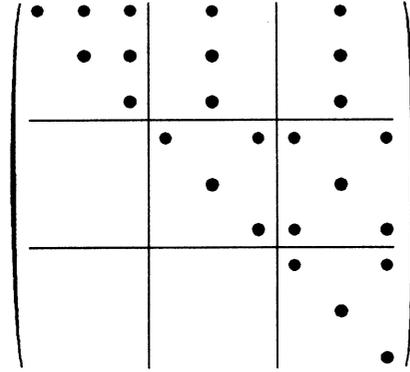
For symmetric tensors such as those representing principal properties, one finds the following, representing the nonzero components for the leading diagonal and for one half of the others.

1.1.4.9.9.1. Triclinic system



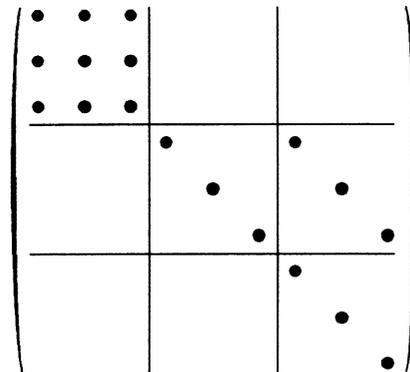
There are 45 independent coefficients.

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 $\bar{3}$

kl	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.

1.1. INTRODUCTION TO THE PROPERTIES OF TENSORS

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

kl	11	22	33	23	31	12	32	13	21
ij									
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.

1.1.4.9.5. Tetragonal system

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

kl	11	22	33	23	31	12	32	13	21
ij									
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 $4/m\bar{m}2, 422, 4mm, \bar{4}2m$

kl	11	22	33	23	31	12	32	13	21
ij									
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.

1.1.4.9.6. Hexagonal and cylindrical systems

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

kl	11	22	33	23	31	12	32	13	21
ij									
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 $6/m\bar{m}2, 622, 6mm, \bar{6}2m; (A_\infty/M)\infty(A_2/M)C, A_\infty\infty A_2$

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

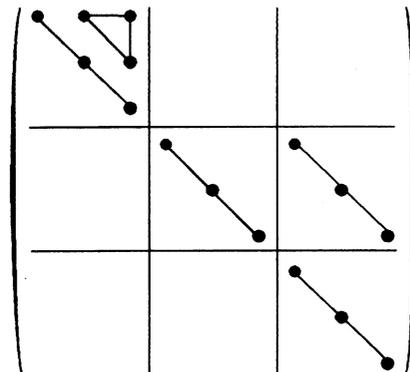
with

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

There are 10 independent components.

1.1.4.9.7. Cubic system

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



with

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

There are 5 independent components.

1. TENSORIAL ASPECTS OF PHYSICAL PROPERTIES

(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 \mathbf{E} (the piezoelectric effect):

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

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 \mathbf{P} when a stress T_{jk} is applied to a crystal:

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

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

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

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

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

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:

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

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:

$$\left(\begin{array}{c|c|c} \mathbf{1} & \mathbf{2} & \mathbf{3} \end{array} \right).$$

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

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

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:

$$\left(\begin{array}{ccc|ccc} 11 & 12 & 13 & 14 & 15 & 16 \\ 21 & 22 & 23 & 24 & 25 & 26 \\ 31 & 32 & 33 & 34 & 35 & 36 \end{array} \right).$$

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**:

$$\left(\begin{array}{c|c} \mathbf{1} & \mathbf{2} + \mathbf{3} \end{array} \right).$$

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

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

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:

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

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

1.1. INTRODUCTION TO THE PROPERTIES OF TENSORS

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

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

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

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, $\bar{3}2$, $3m$, $\bar{6}$, $\bar{6}2m$).

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 :

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

There are 8 independent components.

- (ii) Group m :

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

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 :

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

There are 3 independent components.

- (ii) Group $mm2$:

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

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:

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

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 $\bar{3}2$, twofold axis parallel to Ox_1 :

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

with the same conventions. There are 4 independent components.

- (iii) Group $3m$, mirror perpendicular to Ox_1 :

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

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_∞ :

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

There are 4 independent components.

- (ii) Groups 422 , 622 and $A_\infty \infty A_2$:

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

There is 1 independent component.

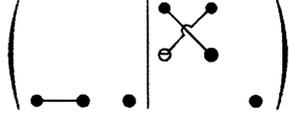
- (iii) Groups $4mm$, $6mm$ and $A_\infty \infty M$:

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

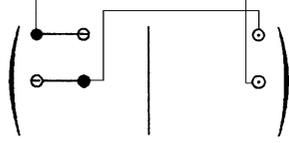
There are 3 independent components.

1. TENSORIAL ASPECTS OF PHYSICAL PROPERTIES

- (iv) Groups $4/m$, $6/m$ and $(A_\infty/M)C$: all the components are equal to zero.
 (v) Group $\bar{4}$:

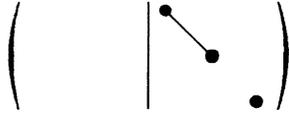


There are 4 independent components.
 (vi) Group $\bar{6} = 3/m$:



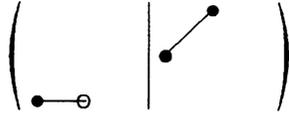
with the same conventions as for group 3. There are 2 independent components.

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

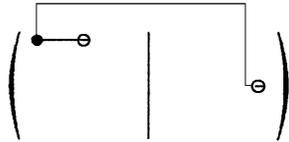


There are 2 independent components.

- (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 $\bar{6}2/m$:

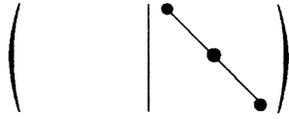


with the same conventions as for group 3. There is 1 independent component.

- (x) Groups $4/m\bar{3}$, $6/m\bar{3}$ 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):

$$S_{ij} = s_{ijkl}T_{kl}, \quad (1.1.4.9)$$

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):

$$S_{ij} = Q_{ijkl}E_kE_l, \quad (1.1.4.10)$$

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:

$$\begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix} = \begin{pmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{pmatrix} \times \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}$$

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

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

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:

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

1.1. INTRODUCTION TO THE PROPERTIES OF TENSORS

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

$$\begin{aligned} s_{ijll} &= s_{jill} \\ s_{ijkl} &= s_{ijlk} = s_{jikl} = s_{jilk}. \end{aligned}$$

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:

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

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

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

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

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

β	1	2	3	4	5	6
α	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:

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

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} :

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

where

$$\begin{aligned} c_{\alpha\beta} &= c_{ijkl} \\ p_{\alpha\beta} &= p_{ijkl}. \end{aligned}$$

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

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

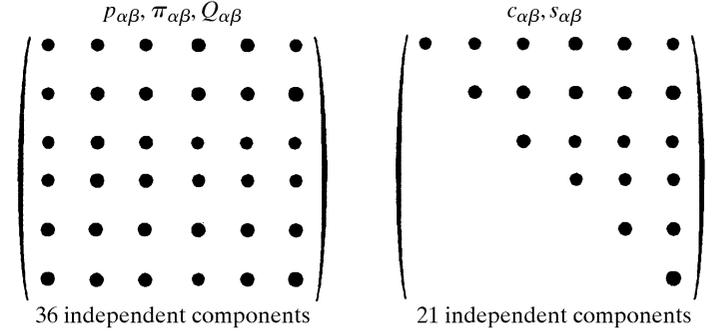
where

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

(iii) *Electrostriction coefficients*, Q_{ijkl} : same relation as for the elastic compliances.

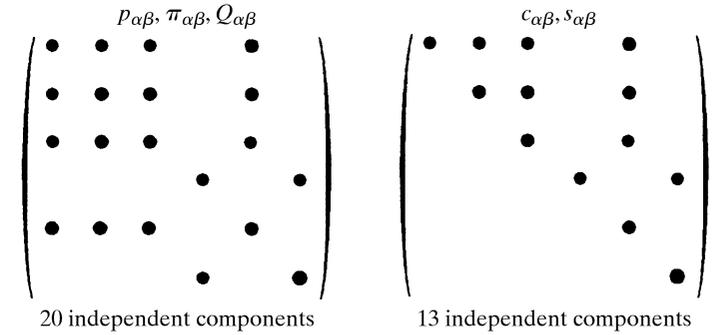
1.1.4.10.6. *Independent components of the matrix associated with a fourth-rank tensor according to the following point groups*

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



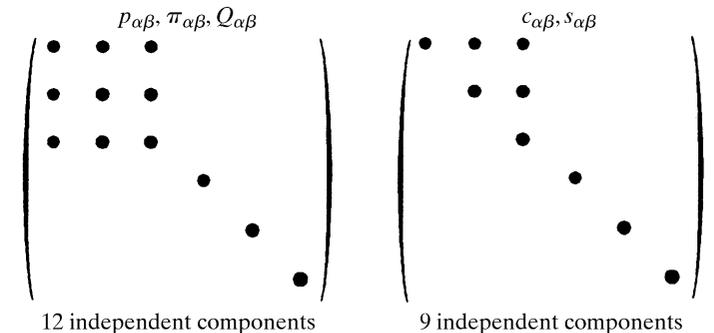
1.1.4.10.6.2. *Monoclinic system*

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



1.1.4.10.6.3. *Orthorhombic system*

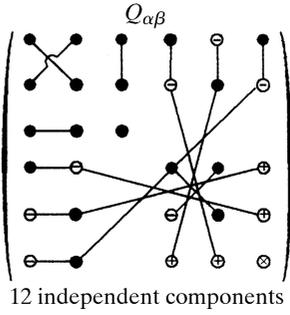
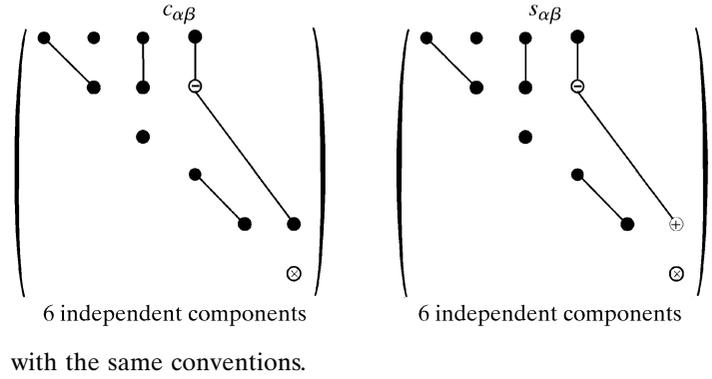
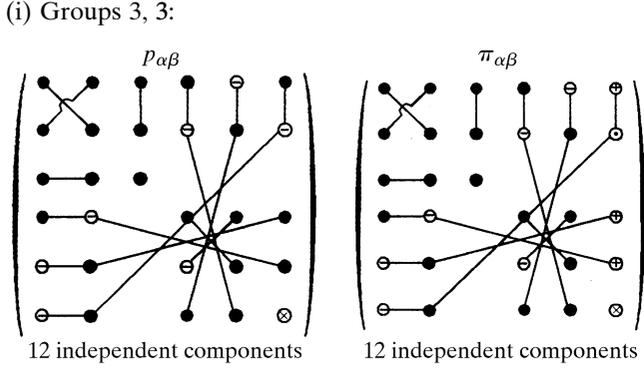
Groups mmm , $2mm$, 222 :



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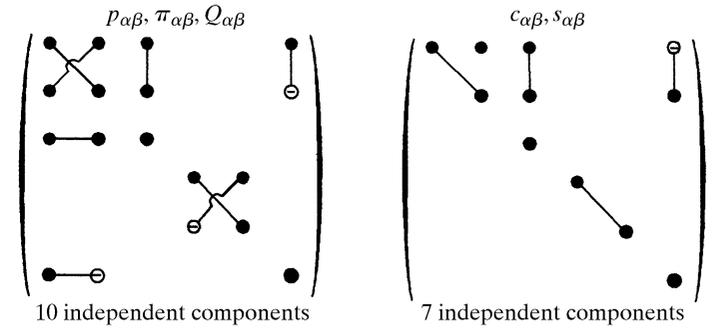
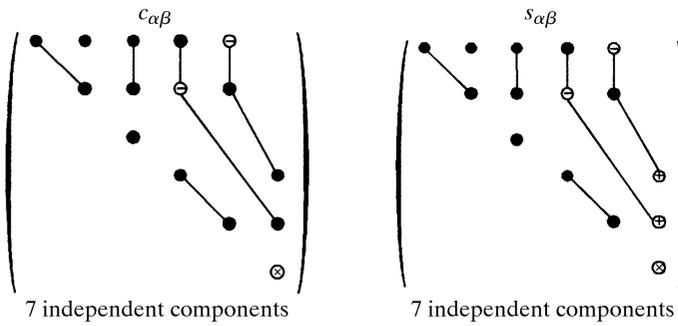
1.1.4.10.6.4. Trigonal system

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

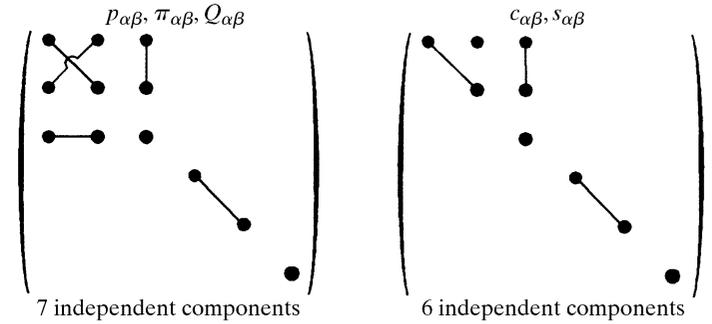


1.1.4.10.6.5. Tetragonal system

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

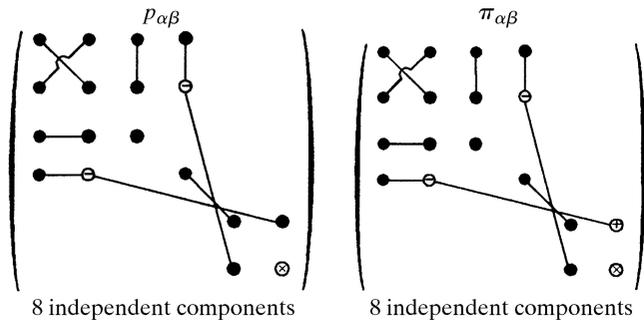


(ii) Groups 422, 4mm, $\bar{4}2m$ and 4/mmm:



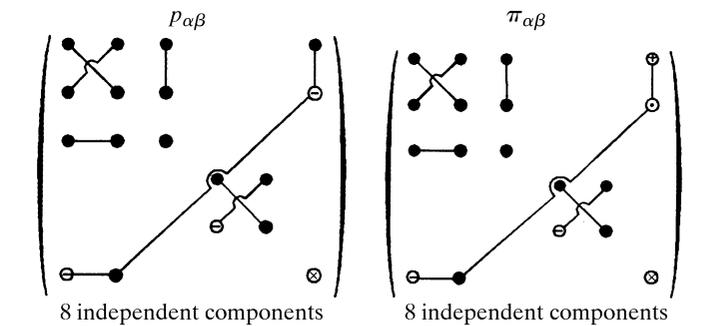
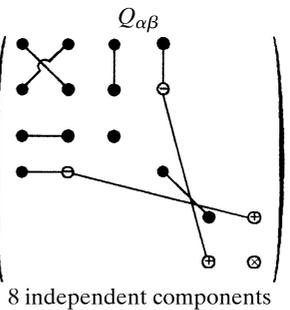
where \ominus is a component numerically equal but opposite in sign to the heavy dot component to which it is linked; \oplus is a component equal to twice the heavy dot component to which it is linked; \odot is a component equal to minus twice the heavy dot component to which it is linked; \otimes is 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, $\bar{3}m$:

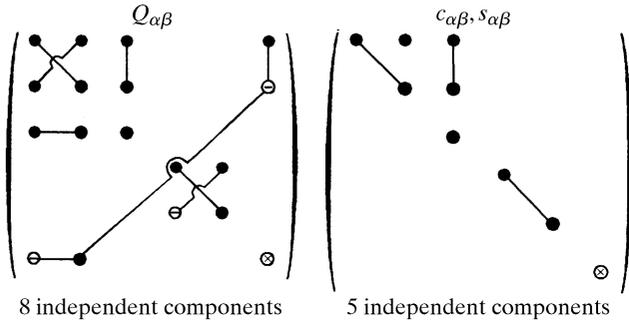


1.1.4.10.6.6. Hexagonal system

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

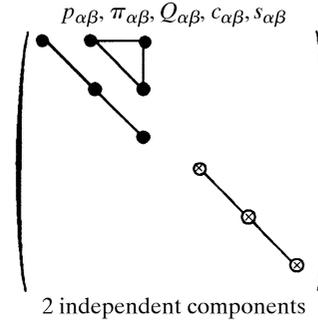


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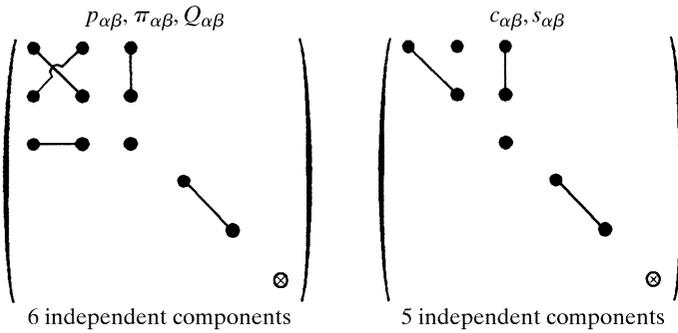


1.1.4.10.6.8. Spherical system

For all tensors



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



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

$$\left(\begin{array}{ccc|ccc|cc} & 122 & 133 & 123 & 131 & & 132 & 121 \\ -121 & & 223 & & 231 & -122 & 232 & -123 \\ -131 & -232 & & -233 & -132 & & -133 & -231 \end{array} \right).$$

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

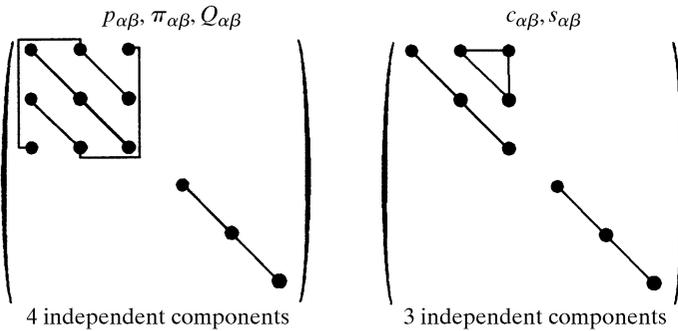
$$g_{kl} = \frac{1}{2}\epsilon_{ijk}g_{ijl}.$$

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 3m:



1.1.4.10.7.1. Independent components according to the following point groups

(i) Triclinic system

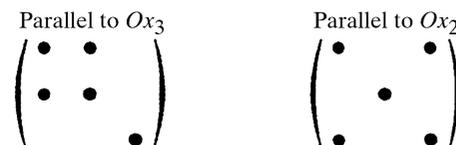
(a) Group 1:



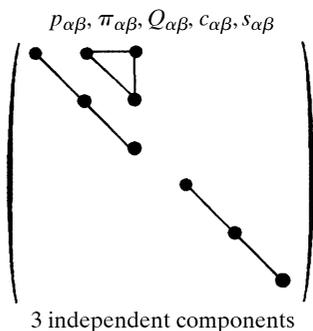
(b) Group $\bar{1}$: all components are equal to zero.

(ii) Monoclinic system

(a) Group 2:

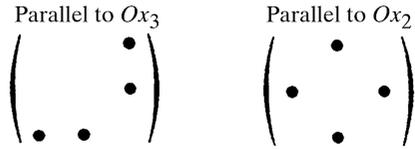


(ii) Groups 432, $\bar{4}3m$ and $m\bar{3}m$:



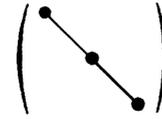
1. TENSORIAL ASPECTS OF PHYSICAL PROPERTIES

(b) Group m :



(v) Cubic and spherical systems

(a) Groups 23, 432 and ∞A_∞ :



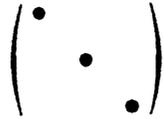
(c) Group $2/m$: all components are equal to zero.

The axial tensor is reduced to a pseudoscalar.

(b) Groups $m\bar{3}$, $43m$, $m\bar{3}m$ and $\infty(A_\infty/M)C$: all components are equal to zero.

(iii) Orthorhombic system

(a) Group 222:

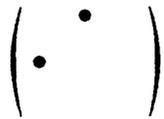


1.1.4.10.7.2. Independent components of symmetric axial tensors according to the following point groups

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)

$$G = g_{ij}\alpha_i\alpha_j,$$

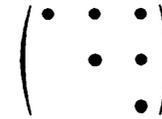
(b) Group $mm2$:



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

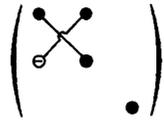
(a) Group 1:



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

(iv) Trigonal, tetragonal, hexagonal and cylindrical systems

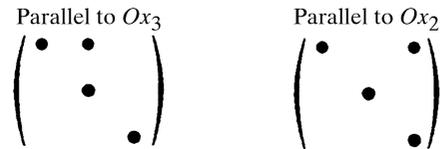
(a) Groups 3, 4, 6 and A_∞ :



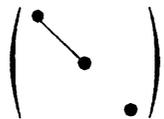
(b) Group $\bar{1}$: all components are equal to zero.

(ii) Monoclinic system

(a) Group 2:



(b) Groups 32, 42, 62 and $A_\infty \infty A_2$:



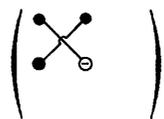
(c) Groups $3m$, $4m$, $6m$ and $A_\infty \infty M$:



(b) Group m :



(d) Group $\bar{4}$:



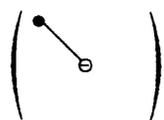
(c) Group $2/m$: all components are equal to zero.

(iii) Orthorhombic system

(a) Group 222:



(e) Group $\bar{4}2m$:



(b) Group $mm2$:

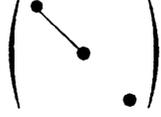


(f) Groups $\bar{3}$, $4/m$, $\bar{6}2m$, $\bar{3}m$, $4/m\bar{m}$ and $6/m\bar{m}$: all components are equal to zero.

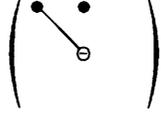
(c) Group mmm : all components are equal to zero.

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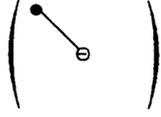
- (iv) *Trigonal, tetragonal and hexagonal systems*
 (a) Groups 3, 32, 4, 42, 6, 62:



- (b) Group $\bar{4}$:

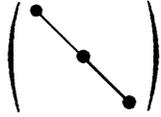


- (c) Group $\bar{4}2m$:



- (d) Groups $\bar{3}$, $3m$, $\bar{3}m$, $4/m$, $4mm$, $4/m\bar{m}m$, $\bar{6}$, $\bar{6}2m$ and $6/mmm$: 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 Sirotnin & 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

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

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

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

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,

$$\begin{aligned} dS_{kl} &= \left[\frac{\partial S_{kl}}{\partial T_{ij}} \right]_{E,\Theta} dT_{ij} + \left[\frac{\partial S_{kl}}{\partial E_n} \right]_{T,\Theta} dE_n + \left[\frac{\partial S_{kl}}{\partial \Theta} \right]_{E,T} \delta\Theta \\ dD_n &= \left[\frac{\partial D_n}{\partial T_{kl}} \right]_{E,\Theta} dT_{kl} + \left[\frac{\partial D_n}{\partial E_m} \right]_{T,\Theta} dE_m + \left[\frac{\partial D_n}{\partial \Theta} \right]_{E,T} \delta\Theta \\ d\sigma &= \left[\frac{\partial \sigma}{\partial T_{ij}} \right]_{E,\Theta} dT_{ij} + \left[\frac{\partial \sigma}{\partial E_m} \right]_{T,\Theta} dE_m + \left[\frac{\partial \sigma}{\partial \Theta} \right]_{E,T} \delta\Theta. \end{aligned}$$

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

$$\left. \begin{aligned} S_{kl} &= (s_{klj})^{E,\Theta} T_{ij} + (d_{kln})^{T,\Theta} E_n + (\alpha_{kl})^{E,T} \delta\Theta \\ D_n &= (d_{nkl})^{E,\Theta} T_{kl} + (\varepsilon_{nm})^{T,\Theta} E_m + (p_n)^{E,T} \delta\Theta \\ \delta\sigma &= (\alpha_{ij})^E T_{ij} + (p_m)^T E_m + (\rho C^{E,T} / \Theta) \delta\Theta. \end{aligned} \right\} \quad (1.1.5.1)$$

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: $(s_{klj})^{E,\Theta}$: 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 \mathbf{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).