International Tables for Crystallography (2006). Vol. D, Section 1.1.3.3, pp. 7–8.

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

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

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

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

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

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

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

1.1.3. Mathematical notion of tensor

1.1.3.1. *Definition of a tensor*

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

1.1.3.1.1. *Linear forms*

A linear form in the space E_n is written

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

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

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

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

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

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

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

1.1.3.1.2. *Tensor product*

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

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

This correspondence possesses the following properties:

(i) it is distributive from the right and from the left;

(ii) it is associative for multiplication by a scalar;

(iii) the tensor products of the vectors with a basis E_n and those with a basis F_p constitute a basis of the product space.

The analytical expression of the tensor product is then

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

One deduces from this that

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

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

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

1.1.3.2. *Behaviour under a change of basis*

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

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

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

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

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

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

As the decomposition is unique, one obtains

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

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

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

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

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

so that

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

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

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

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

1.1.3.3. *Operations on tensors*

1.1.3.3.1. *Addition*

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

1.1.3.3.2. *Multiplication by a scalar*

This is a particular case of the tensor product.

1.1.3.3.3. *Contracted product, contraction*

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

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

$$t'^j_i = A^j_p B^q_i t^p_q.$$

Now consider the quantity t'^i_i derived by applying the Einstein convention ($t'^i_i = t'^1_1 + t'^2_2 + t'^3_3$). It follows that

$$t'^i_i = A^i_p B^q_i t^p_q = \delta^q_p t^q_q$$
$$t'^i_i = t^p_p.$$

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

The *contraction* consists therefore of equalizing a covariant index and a contravariant index, and then in summing over this index. Let us take, for example, the tensor t'^{jk}_i. Its contracted form is t'^{ik}_i, which, with a change of basis, becomes

$$t'^{ik}_i = A^k_p t^{qp}_q.$$

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

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

$$O^1_1 + O^2_2 + O^3_3 = O^i_i.$$

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

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

$$p^{jk}_i = t^j_i z^k.$$

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

$$p^{ji}_i = t^j_i z^i.$$

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

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

$$t^j_i = x_i y^j.$$

After contraction, we get the scalar product:

$$t^i_i = x_i y^i.$$

1.1.3.4. *Tensor nature of physical quantities*

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

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

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

$$D^1 = \varepsilon^1_1 E^1 + \varepsilon^1_2 E^2 + \varepsilon^1_3 E^3.$$

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

$$D^i = \varepsilon^i_j E^j \qquad (1.1.3.3)$$

using the Einstein convention.

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

$$D^i x_i = \varepsilon^i_j E^j x_i.$$

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

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

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

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

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

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

1.1.3.5. *Representation surface of a tensor*

1.1.3.5.1. *Definition*

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

$$t'_{1111\ldots} = t_{ijkl\ldots} B^i_1 B^j_1 B^k_1 B^l_1 \ldots,$$

where the B^i_1, $B^j_1, \ldots$ are the direction cosines of that direction with respect to the axes of the orthonormal frame.

The *representation surface* of the tensor is the polar plot of $t'_{1111\ldots}$.

1.1.3.5.2. *Representation surfaces of second-rank tensors*

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