3 Definitions

3.1 Properties

The physical phenomena of matter are made apparent in experiments and their quantitative formulation in measurements. The results of such measurements can often lead to direct statements concerning the so-called properties of the given substance. We now want to look more closely at the term property. For this purpose, we imagine those actions, embracing the group of independent or *inducing quantities*, which we can arbitrarily perform on a probe. Let these be specified by the symbol $A_{j'j''j'''\ldots}$, or in short notation A_j, where the indices j', j'', and so on are introduced to more precisely characterize the quantities. Such independent quantities are, for example, volume, temperature, temperature gradients, hydrostatic pressure, pressure gradients, general mechanical stress states, velocity, rotational velocity, electric, and magnetic field strengths.

The inducing quantities give rise to effects which we measure with the aid of dependent or *induced quantities* $B_{i'i''i'''\ldots}$, in short notation B_i. Examples for B_i are: caloric heat content, mechanical deformation, heat flow density, mass flow density, electric current density, electric polarization, and magnetization. The relationship between inducing and induced quantities is described by

$$B_i = f_{i;jkl\ldots}(A_j, A_k, A_l, \ldots).$$

Consequently, the function $f_{i;jkl\ldots}$ specifies those properties of the body which under the action of the quantities A_j, A_k, A_l, and so on produce the quantities B_i. This concept for the definition of properties has been found to be sufficient for most macroscopic phenomena as we shall see in the following.

There also exists a further group of properties, which are derived as functions $g(f_1, f_2, \ldots)$ of certain f_i (here, e.g., f_1, f_2 ...) such as light velocity and sound velocity. We shall call These properties *derived properties*. Sometimes the question has to be settled as to whether the role of the inducing and induced quantities, which may be assigned to each other in pairs, e.g., mechan-

Physical Properties of Crystals. Siegfried Haussühl.

ISBN: 978-3-527-40543-5

ical stress and mechanical deformation or electric field strength and current density, is interchangeable. The formal description often allows such inversions; however, the physical realization of the inversion is often not easy to achieve, as one knows from the example of mechanical deformation and mechanical stress. We will return to this matter in detail in the discussion of actual properties.

As a simple example for the concept of inducing and induced quantities let us consider *specific heat* and *electric conductivity*. The specific heat C_p (per g, at constant pressure) connects an arbitrary temperature rise ΔT, as an inducing quantity, to the consequent appearance of an increase in the caloric capacity ΔQ_p (per g, at constant pressure) according to

$$\Delta Q_p = C_p \Delta T.$$

Here, f is a linear function of the independent variable ΔT. This association is approximately valid in a small temperature interval. An exchange of inducing and induced quantities is not only formally but also physically feasible.

The electrical conductivity s establishes the connection between electric charge current density $\boldsymbol{I}$ (unit: charge per s and mm^2) and the electric field strength $\boldsymbol{E}$ as the inducing quantity according to

$$\boldsymbol{I} = s\boldsymbol{E}.$$

This form of Ohm's law is approximately correct for isotropic, i.e., directionally independent, conductivity. With crystals of lower symmetry, as e.g., arsenic, antimony or bismuth (PSG $\bar{3}$m) or with $LiIO_3$ (PSG 6) one observes in the direction of the threefold or sixfold axis other values of electric conductivity as in the direction perpendicular to these. Related to the crystal-physical system, the conductivity along the three- or sixfold axis is described by $I_3 = s_{33}E_3$ and perpendicular to these by $I_1 = s_{11}E_1$. We thus find an anisotropy, represented by the introduction of the mutually independent components of the electric field E_i and of the current density vector I_i ($i = 1, 2, 3$). We will discuss in detail the question of how the anisotropy looks like in general, i.e., which relationship exists between $\boldsymbol{I}$ and $\boldsymbol{E}$ in an arbitrary direction.

The functions f and therefore the properties are divided into two groups:

I. Tensor Properties. A multilinear relationship exists between B_i and the A_j of the type

$$B_i = f^0_{i;j} A_j + f^0_{i;jk} A_j A_k + f^0_{i;jkl} A_j A_k A_l + \cdots$$

(One sums according to the summation convention.) The $f^0_{i;jkl\ldots}$ are constant coefficients and all nonaffected inducing quantities are held constant. This representation corresponds to a Taylor series in B_i according to

$$B_i = \sum_\nu \frac{1}{\nu!} \frac{\partial^\nu B_i}{\partial A_j \partial A_k \cdots} A_j A_k \cdots,$$

with the characteristic that no constant term is present. The expansion occurs at the zero value of all A_j.

The coefficients $f^0_{i;jkl\ldots}$ with fixed indices $jkl\cdots$ represent a certain property. In the case of a single index j we are dealing with a property of the first order, with index pairs jk we are dealing with properties of the second order, and so on. Many mechanical, electrical, optical, and thermal properties, also those of a very complicated nature, belong to the tensor properties.

II. Nontensor Properties. Here, the relationship between inducing and induced quantities is more complicated. Nontensor properties are, e.g., growth properties, rate of dissolution (etching behavior), boundary surface properties, plasticity, abrasive hardness, scratch hardness, and properties connected with energetic activation thresholds, e.g., in emission and absorption processes.

3.2 Reference Surfaces and Reference Curves

Many properties, especially the tensor properties, possess an anisotropy, which can be represented by a surface in space.

In the case of a simple directional dependence, the reference surface furnishes an overview of the complete anisotropy. We obtain the reference surface as the entirety of the end points of radius vectors $\boldsymbol{r}$, spreading from a fixed point, with lengths equal to the value of the property for the given direction. As an example we mention the *rate of dissolution* which describes the etching behavior on a given face of a crystal in a distinct solvent (see Fig. 3.1; the measurement method is described in Section 6.2.

In the same manner as with the rate of dissolution, one can also represent, e.g., abrasive strength, indentation hardness (a measure for the plasticity), and the tensile strength of thin cylinders with the aid of a simple reference surface. A special reference surface is generated by a freely growing crystal through its outer boundary surface, which represents the mean velocity of crystallization in any direction.

If there exists, for each measurement direction, several values of the given property, then one gets a multishell reference surface. For example, one needs for the representation of the velocity of light in crystals a double-shelled reference surface because for each propagation direction two different values of the velocity of light exist. In the case of sound velocity, a triple-shell surface is required because for each propagation direction three different values of sound velocity are possible. We will handle these and other examples in more detail later.

For some properties, in which several directions simultaneously come into play as, for example, with sawing velocity and scratch hardness, a compli-

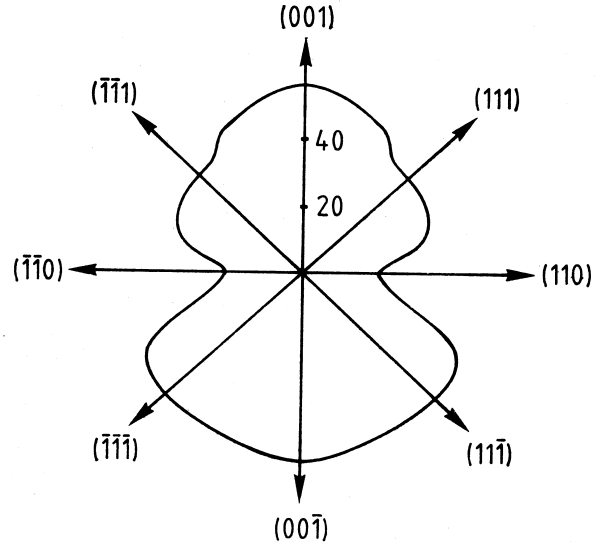

Figure 3.1 Anisotropy of dissolution velocity of $Sr(HCOO)_2 \cdot 2H_2O$, PSG 22, in water at 293 K. The radial distances give the loss in weight in mg per 100 ml H_2O in directions within the zone $[1\bar{1}0]$. A distinct minimum is observed on the principal growth faces $\{110\}$. The anisotropy reflects the symmetry of the twofold axis along $[001]$. The lack of a center of inversion is immediately recognizable.

cated representation in the form of reference curves must be chosen, because the measurement results depend not only on the orientation of the crystal face but also on the cutting direction of the saw or the direction of scratching (Section 6.3).

3.3 Neumann's Principle

The consequences of crystal symmetry on the physical properties, in which the influence of boundaries can be neglected, are governed by a fundamental postulate of crystal physics, known as Neumann's principle (F. Neumann, 1798–1895):

"The space symmetry of the physical properties of a crystal cannot be less than the structural symmetry of the crystal."

As a justification, it suffices to note that the given property is a consequence of the atomic arrangement of the lattice particles and their bonding, i.e., the electronic states. Other reasons for the occurrence of the properties do not exist, as long as we look at the empty space, in which the material is embedded,

as an intrinsically isotropic medium. This assumption is essentially fulfilled for our purposes. In all macroscopic properties, the point group symmetry replaces the position of the structural symmetry described by the space group symmetry. This is due to the fact that translation symmetry is macroscopically not immediately recognizable and the special operations of screw axes and glide mirror planes, in the macroscopic sense, act as ordinary symmetry axes or mirror planes. From Neumann's principle we learn immediately that the reference surfaces must at least possess the point symmetry group of the given crystal as long as boundary-independent properties are considered. The mathematical formulation for this fact is as follows: the reference surfaces are invariant under the transformations of the point symmetry group.

Thus each continuous reference surface is to be approximated to an arbitrary degree by symmetry-fitted fundamental polynomials of the given symmetry group (Exercise 2). In order to make use of this relationship, it is important, as far as possible, to define the properties so that they are boundary independent. Furthermore, we always assume that the observed properties fulfill this requirement if no special indications are given for another situation. When nothing else is said, we also assume that the properties of the crystal, and therefore also their intrinsic symmetry are not measurably changed by the action of the inducing quantities. Thus for the description of the phenomena we will also view the crystal-physical reference system as fixed and invariable.

3.4 Theorem on Extreme Values

In directions of symmetry axes with $n \geq 3$ the properties take on relative extreme values, i.e., in all sufficiently adjacent directions we find either larger or smaller values of the given properties, except for the isotropic case which does not concern us here. In directions of twofold axes, the properties take on either extreme values or saddle point values, i.e., the reference surface possesses at such points along the principal curvature lines perpendicular to one another relative extreme values that can also be of a different character (maximum or minimum). In all directions within a symmetry plane, each property takes on a relative extreme value when passing through the principal curvature line perpendicular to the symmetry plane. There is no general rule for extreme values in other directions or the position of absolute extreme values.

As proof we imagine that the reference surface is differentiable to sufficient order. Then in each point there exist two defined principal curvatures, a maximum and a minimum. We now replace the reference surface by an elliptic or hyperbolic paraboloid tangential to the surface in the given point and with principal curvatures corresponding to those of the surface (*Dupin indicatrix*).

In the coordinate system, whose basic vectors $\boldsymbol{e}'_1$ and $\boldsymbol{e}'_2$ are given by the tangents along the directions of principal curvature ($\boldsymbol{e}'_3$ is perpendicular to the tangential plane), the paraboloid is given by

$$ax'^2_1 + bx'^2_2 + cx'_3 = 0.$$

In the case of n-fold axes with $n \geq 3$, the paraboloid has the form of a rotation paraboloid ($a = b$). All points of the reference surface in a certain neighborhood of the intercept point of an n-fold axis lie approximately on the paraboloid, that again, in the point of contact, is to be approximated by a sphere of a radius corresponding to the principal curvature. This radius is either smaller or larger than the length of the radius vector of the reference surface, i.e., the radius vector leads either to a maximum or a minimum. In the intercept point of a twofold axis, the axis $\boldsymbol{e}'_3$ of the Dupin indicatrix runs parallel to the twofold axis. This is compatible with the existence of an extreme value or a saddle point. For directions within a symmetry plane, the vectors $\boldsymbol{e}'_1$ and $\boldsymbol{e}'_2$ of the Dupin indicatrix lie parallel and perpendicular, respectively, to the symmetry plane. Thus it follows, as stated, that when passing through the principal curvature line perpendicular to the symmetry plane there must appear a relative extreme value for all directions in the symmetry plane. Furthermore, in the directions within a symmetry plane there exist an even quantity of relative extreme values with the same number of maxima and minima. There exists at least one maximum and one minimum.

3.5 Tensors

As previously mentioned, many important physical properties can be described by *tensors*. In the next few sections we will get to know some properties of tensors, which will be extremely useful for further work. The beginner should familiarize himself with this mathematical tool as soon as possible. Often the endeavor to evoke a picture of the nature of tensors is futile and leads to a certain aversion. For this reason, such attempts should not be stimulated at the beginning. Rather it is recommended, at first only to pay attention to the definitions that follow and the rules of calculation resulting from these. We will then derive those quantities which provide us a useful conception of tensors. As a first step we will introduce tensors on the basis of their transformation properties. For this purpose we will recapitulate the behavior of basic vectors and coordinates of the position vector when changing a reference system. The introduction of a new reference system with the basic vectors $\boldsymbol{a}'_i$ takes place advantageously with the help of the transformation matrix (u_{ij}) which generates the new basic vectors from the old according to $\boldsymbol{a}'_i = u_{ij}\boldsymbol{a}_j$. The reverse transformation as well as the transformation of the position vec-

Table 3.1 Formulae for the transformation into a new reference system. The coordinates of the position vector in the reciprocal system are designated by x_i^* for the sake of uniformity. In crystallography normally the symbols h_i are used. (U_{ij}), the inverse matrix of (u_{ij}), is obtained by $U_{ij} = (-1)^{i+j} A_{ji}/|u_{ij}|$, where A_{ji} is the adjunct determinant resulting from the transformation matrix after dropping the jth row and ith column. $|u_{ij}|$ is the determinant of the transformation matrix.

$\boldsymbol{a}_i' = u_{ij}\boldsymbol{a}_j$	$\boldsymbol{a}_i = U_{ij}\boldsymbol{a}_j'$	$x_i' = U_{ji}x_j$	$x_i = u_{ji}x_j'$
$\boldsymbol{a}_i^{*\prime} = U_{ji}\boldsymbol{a}_j^*$	$\boldsymbol{a}_i^* = u_{ji}\boldsymbol{a}_j^{*\prime}$	$x_i^{*\prime} = u_{ij}x_j^*$	$x_i^* = U_{ij}x_j^{*\prime}$

tors in the old and new systems and also in the associated reciprocal systems is compiled in Table 3.1 (refer to Section 1.6 for the derivation of the formulae).

Quantities that transform as the basic vectors of the initial system with the matrix (u_{ij}) are called covariant, and those that transform as the basic vectors of the associated reciprocal system with the matrix (U_{ji}) are called contravariant. The coordinates of the position vector in the basic system are the contravariant coordinates, and the coordinates of the same position vector in the reciprocal system are the covariant coordinates. A simplification of the situation occurs when Cartesian reference systems are used. We consider the transformation $\boldsymbol{e}_i' = u_{ij}\boldsymbol{e}_j$ with the reverse $\boldsymbol{e}_i = U_{ij}\boldsymbol{e}_j'$. Then we have

$$\boldsymbol{e}_i' \cdot \boldsymbol{e}_j = u_{ij} = \boldsymbol{e}_j \cdot \boldsymbol{e}_i' = U_{ji}.$$

Thus in Cartesian systems, covariant and contravariant transformations are not distinguishable. This is a good reason to prefer Cartesian reference systems in practical crystal physics. Transformation matrices with the above properties are called unitary ($\boldsymbol{U} = (\boldsymbol{U}^{-1})^T$).

We now consider the ensembles of quantities $t_{ijk\ldots s}$, where each individual attribute, labeled by the index positions i, j, k $\ldots$ s, runs through a certain range of values. An example for such quantities is index cards of a file system, as used, for example in animal husbandry. The first index is provided, let us say, for the date of birth, the second for gender, the third for the breed, and so on. Under all these varieties there exists a marked group, whose members, also called elements, exhibit a special internal relationship. We are dealing with tensors. The individual quantities $t_{ijk\ldots s}$ are called *tensor components*. We specify the ensemble of components, the tensors, by $\{t_{ijk\ldots s}\}$. If the tensor components possess m index positions, then we are dealing with a *tensor of the mth rank*. The range of values of all indices covers the numbers $1, 2, 3, \ldots, n$, where n is the dimension of the associated space. The tensors are thus assigned to an n-dimensional space, which, for example, is spanned by the Cartesian vectors $\boldsymbol{e}_i$ $(i = 1, 2, \ldots, n)$. The tensors distinguish themselves from the other quantities by their transformation behavior when changing the reference system. The definition of tensors in this way may, at first, seem artificial. We will see, however, that just this property of tensors is of fundamental importance for

all further work, especially for direct applications. The definition reads as follows: Ensembles, whose components $t_{ijk\ldots s}$ transform like the corresponding coordinate products during a change of the reference system, are tensors. With a covariant transformation of all index positions, the components $t_{ijk\ldots s}$ are assigned to the product $x_i^* x_j^* x_k^* \cdots x_s^*$, and with a contravariant transformation they are assigned to the product $x_i x_j x_k \cdots x_s$. In principle, a certain transformation behavior (covariant or contravariant) is allowed for each individual index position. When changing the reference system $t_{ijk\ldots s}$ converts in

$$t'_{ijk\ldots s} = u_{ii^*} u_{jj^*} u_{kk^*} \cdots u_{ss^*} t_{i^*j^*k^*\ldots s^*}$$

with a covariant transformation and to

$$t'_{ijk\ldots s} = U_{i^*i} U_{j^*j} U_{k^*k} \cdots U_{s^*s} t_{i^*j^*k^*\ldots s^*}$$

with a contravariant transformation.

One sums over all indices $i^*, j^*, k^*, \ldots, s^*$ from 1 to n. This results directly from

$$x'_i x'_j x'_k \cdots x'_s = U_{i^*i} U_{j^*j} U_{k^*k} \cdots U_{s^*s} x_{i^*} x_{j^*} x_{k^*} \cdots x_{s^*}$$

and the corresponding expression for the covariant coordinate product. The indices primed with a star only serve to distinguish the indices and are not to be confused with those used to specify the quantities of the reciprocal system. In mixed variant transformations, the component of the corresponding transformation matrix is to be inserted for each index position.

The inverse transformation is carried out in an analogous manner. We have

$$t_{ij\ldots s} = U_{ii^*} U_{jj^*} \cdots U_{ss^*} t'_{i^*j^*\ldots s^*}$$

for the covariant transformation and

$$t_{ij\ldots s} = u_{i^*i} u_{j^*j} \cdots u_{s^*s} t'_{i^*j^*\ldots s^*}$$

for the contravariant transformation.

If we work in Cartesian reference systems, which we will do in the following almost without exception, no difference between both transformation methods exists. Moreover, the introduction of general coordinates, such as cylindrical or polar coordinates, brings advantages only in exceptional cases.

In practical work we are always confronted with the question of whether a tensorial connection exists between inducing and induced quantities. For example, are we dealing with tensor components with quantities s_{ij} obeying a linear relationship $I_i = s_{ij} E_j$ between the components of the current density vector and the electric field? Situations like these can be elegantly handled with the help of the following theorem.

3.6 Theorem on Tensor Operations

If in an arbitrary reference system the mth rank tensor $p_{ij\ldots s}$ is connected to the nth rank tensor $q_{\alpha\beta\ldots\sigma}$ according to

$$p_{ij\ldots s} = r_{ij\ldots s;\alpha\beta\ldots\sigma} q_{\alpha\beta\ldots\sigma}$$

by the quantities $r_{ij\ldots s;\alpha\beta\ldots\sigma}$, which carry a total of $(m+n)$ index positions, then the ensemble $\{r_{ij\ldots s;\alpha\beta\ldots\sigma}\}$ also represents a tensor. The proof is as follows: We imagine having performed a transformation in a Cartesian basic system with the basic vectors $\boldsymbol{e}'_i = u_{ii^*}\boldsymbol{e}_{i^*}$. The relation given above then reads

$$p'_{ij\ldots s} = r'_{ij\ldots s;\alpha\beta\ldots\sigma} q'_{\alpha\beta\ldots\sigma}.$$

We have

$$p'_{ij\ldots s} = u_{ii^*} u_{jj^*} \cdots u_{ss^*} p_{i^*j^*\ldots s^*}.$$

For $p_{i^*j^*\ldots s^*}$ we insert the above expression and obtain after exchanging indices

$$p'_{ij\ldots s} = u_{ii^*} u_{jj^*} \cdots u_{ss^*} r_{i^*j^*\ldots s^*;\alpha^*\beta^*\ldots\sigma^*} q_{\alpha^*\beta^*\ldots\sigma^*}.$$

Now we substitute the components $q_{\alpha^*\beta^*\ldots\sigma^*}$ with the help of the inverse transformation by

$$u_{\alpha\alpha^*} u_{\beta\beta^*} \cdots u_{\sigma\sigma^*} q'_{\alpha\beta\ldots\sigma},$$

and get

$$p'_{ij\ldots s} = u_{ii^*} u_{jj^*} \cdots u_{ss^*} u_{\alpha\alpha^*} u_{\beta\beta^*} \cdots u_{\sigma\sigma^*} r_{i^*j^*\ldots s^*;\alpha^*\beta^*\ldots\sigma^*} q'_{\alpha\beta\ldots\sigma}.$$

Comparing this with the expression given above in an arbitrary Cartesian reference system yields

$$r'_{ij\ldots\sigma} = u_{ii^*} u_{jj^*} \cdots u_{\sigma\sigma^*} r_{i^*j^*\ldots\sigma^*}.$$

This relation is nothing else but the transformation rule for tensors. Thus the $r_{ij\ldots\sigma}$ are in fact components of a tensor.

Let us now consider some examples of such tensor connections which will illustrate the special usefulness of the theorem just discussed.

We will proceed with increasing rank and distinguish between the group of inducing and induced quantities and the group of tensor properties.

As a general example, consider the Taylor expansion of a scalar function

$$F(\boldsymbol{x}) = \sum_{(ij\ldots s),n} \frac{1}{n!} \frac{\partial^n F}{\partial x_i \partial x_j \cdots \partial x_s} x_i x_j \cdots x_s$$

about the point $\boldsymbol{x} = 0$. As is well known, one sums over all permutations of the indices for each n. If we go over to a new reference system $F(\boldsymbol{x}) = F(\boldsymbol{x}')$ is preserved. On the left-hand side we have a zero-rank tensor, a quantity that does not change with a transformation. The individual differential quotients for each fixed n are tensor components because they are connected with the coordinate products $x_i x_j \cdots x_s$ which themselves represent tensor components.

It is obvious that the coordinate products of a vector or arbitrary vectors are also tensor components, likewise the differential quotients of tensors with respect to the components of other tensors, as e.g., the differential quotients with respect to time, temperature, pressure or with respect to the components of the position vector, and so on. Furthermore, the products of components of two or more tensors also represent tensor components just as the differential quotients of components of a vector or of different vectors or tensors, respectively. A further possibility of creating tensors from existing tensors is the operation of tensor contraction. Let there be two tensors $\{a_{ij\ldots rs}\}$ and $\{b_{\alpha\beta\ldots\rho\sigma}\}$ of arbitrary rank. The connection of these tensors according to

$$c_{ij\ldots r;\alpha\beta\ldots\rho} = a_{ij\ldots rs} b_{\alpha\beta\ldots\rho s},$$

which contains a summation over a common index position (or in the general case, several common index positions: multiple contraction), leads also to a tensor, whose rank for each summation position is two less than the sum of the ranks of both initial tensors. The proof for a simple contraction is based upon the transformation behavior. We write on the right-hand side of the above equation the inverse transformations

$$a_{ij\ldots rs} = u_{i^*i} u_{j^*j} \cdots u_{r^*r} u_{s^*s} a'_{i^*j^*\ldots r^*s^*}$$

and

$$b_{\alpha\beta\ldots\rho s} = u_{\alpha^*\alpha} u_{\beta^*\beta} \cdots u_{\rho^*\rho} u_{\sigma^*s} b'_{\alpha^*\beta^*\ldots\rho^*\sigma^*}$$

and get

$$c_{ij\ldots r\alpha\beta\ldots\rho} = a'_{i^*j^*\ldots r^*s^*} b'_{\alpha^*\beta^*\ldots\rho^*\sigma^*} u_{i^*i} u_{j^*j} \cdots u_{r^*r} u_{\alpha^*\alpha} u_{\beta^*\beta} \cdots u_{\rho^*\rho} (u_{s^*s} u_{\sigma^*s}).$$

The expression in the brackets represents a summation over s. When transforming from Cartesian systems, it takes on the value 0 for $s^* \neq \sigma^*$ and the value 1 for $s^* = \sigma^*$. Thus

$$c_{ij\ldots r\alpha\beta\ldots\rho} = a'_{i^*j^*\ldots r^*s^*} b'_{\alpha^*\beta^*\ldots\rho^*s^*} u_{i^*i} u_{j^*j} \ldots u_{r^*r} u_{\alpha^*\alpha} u_{\beta^*\beta} \ldots u_{\rho^*\rho}.$$

This is the formula for the inverse transformation of the tensor components $c'_{i^*j^*\ldots\rho^*}$; thus the contraction process results in a new tensor. The proof is carried out in a corresponding manner for the case of several contractions with

arbitrarily chosen index positions. If one works in a non-Cartesian system, the index positions, over which one sums, must have different transformation behavior (covariant or contravariant) in both tensors $\{a\}$ and $\{b\}$. The contraction operation plays an important role in the generation of invariants which we will consider later.

We should note that the theorem on tensor operations represents nothing else but multiple contraction operations. The formulation of the problem, however, is different to the contraction case just discussed.

We now come to concrete examples which will be discussed in detail in later sections. For the sake of brevity, we will specify inducing or induced quantities with I and properties with II.

Zero-Rank Tensors (Scalars)

I: Temperature, pressure, volume, electrical potential, as well as differences and differential quotients of these quantities,

II: Specific weight ρ, specific heat C_p and other energy densities, all mean values of anisotropic properties in space, e.g., mean speed of light, mean abrasive strength, mean electrical conductivity; scalar invariants; all properties of isotropic substances.

First-Rank Tensors (Vectors)

I: Position vector $\boldsymbol{x}$, differential quotient of vectors with respect to scalars (e.g., velocity, acceleration), angular vector $\boldsymbol{u}$, impulse, angular momentum $\boldsymbol{L}$, gradients of scalar fields (temperature, pressure), electric field strength $\boldsymbol{E}$, magnetic field strength $\boldsymbol{H}$, current density vectors (heat, charge, mass), electric moment, magnetic moment. (Explanation: the gradient of a scalar function F is the vector grad $F(x) = \frac{\partial F}{\partial x_i}\boldsymbol{e}_i$).

II: Pyroelectric effect $\{\pi_i\}$: Change in electric polarization $\boldsymbol{P}$ induced by a change in temperature ΔT according to $\Delta P_i = \pi_i \Delta T$. Since the left side represents a tensor of rank 1 and ΔT is a scalar, the quantities π_i are components of a tensor of rank 1. A crystal possessing such a property is assigned a fixed vector. Similarly, there exists a pyromagnetic effect and the piezoelectric effect by a change in the hydrostatic pressure Δp according to $\Delta P_i = q_i \Delta p$.

Second-Rank Tensors

I: Products of components of a vector or components of two vectors $\{x_i x_j\}$ or $\{x_i y_j\}$; differential quotients of components of a vector $\{\frac{\partial E_i}{\partial x_j}\}$ (vector gradient) and differential quotients of types $\{\frac{\partial^2 F}{\partial x_i \partial x_j}\}$, $\{\frac{\partial^2 F}{\partial x_i \partial y_j}\}$, $\{\frac{\partial F}{\partial t_{ij}}\}$; deformation tensor $\{\varepsilon_{ij}\}$ and mechanical stress tensor $\{\sigma_{ij}\}$; quadrupole moment; differential quotients of second-rank tensors with respect to a scalar.

II: *Thermal Conductivity* $\{\lambda_{ij}\}$: $Q_i = -\lambda_{ij}(\text{grad}\, T)_j$; $\boldsymbol{Q}$ is the heat current density vector. In this case, as with some of the following examples, the combination of two vectors is by means of a second-rank tensor $\{\lambda_{ij}\}$.

Electrical Conductivity $\{s_{ij}\}$: $I_i = s_{ij}E_j = -s_{ij}(\text{grad}\, U)_j$; $\boldsymbol{I}$ is the charge density vector, U the electric potential.

Mass Permeability $\{q_{ij}\}$: $S_i = -q_{ij}(\text{grad}\, p)_j$; $\boldsymbol{S}$ is the mass density vector.

Dielectricity $\{\epsilon_{ij}\}$: $D_i = \epsilon_{ij}E_j$; $\boldsymbol{D}$ is the vector of the electric displacement, $\boldsymbol{E}$ the vector of the electric field strength.

Magnetic Permeability $\{\mu_{ij}\}$: $B_i = \mu_{ij}H_j$; $\boldsymbol{B}$ is the vector of magnetic induction, $\boldsymbol{H}$ the vector of magnetic field strength.

Thermal Expansion $\{\alpha_{ij}\}$: $\varepsilon_{ij} = \alpha_{ij}\Delta T$; the mechanical deformations ε_{ij} are proportional to the scalar ΔT. Thus $\{\alpha_{ij}\}$ is also a second-rank tensor, since $\{\varepsilon_{ij}\}$ is a tensor as will be shown later.

Volta Striction $\{\beta_{ij}\}$: $\varepsilon_{ij} = \beta_{ij}\Delta U$; this is analogous to thermal expansion. ΔU is the electrical potential difference.

Linear Compressibility at Hydrostatic Pressure $\{K_{ij}\}$: $\varepsilon_{ij} = K_{ij}\Delta p$; this is also analogous to thermal expansion. Δp is the hydrostatic pressure difference.

Moment of Inertia $\{\Theta_{ij}\}$: $L_i = \Theta_{ij}u_j$; $\boldsymbol{u}$ is the angular vector, $\boldsymbol{L}$ the angular momentum vector.

First-Order Displacement Vector $\{v_{ij}\}$: $\xi_i = v_{ij}x_j$; $\boldsymbol{\xi}$ is the displacement vector describing the displacement of the end point of $\boldsymbol{x}$.

Third-Rank Tensors

I: Coordinate products $\{x_ix_jx_k\}$ or $\{x_iy_jz_k\}$ and the differential quotients of the types

$$\left\{\frac{\partial^3 F}{\partial x_i \partial x_j \partial x_k}\right\}, \left\{\frac{\partial^2 E_i}{\partial x_j \partial x_k}\right\}, \left\{\frac{\partial E_i}{\partial t_{jk}}\right\}, \text{ and } \left\{\frac{\partial E_i E_j}{\partial x_k}\right\}$$

and so on.

II. *Piezoelectric Tensor* $\{d_{ijk}\}$: $P_i = d_{ijk}\sigma_{jk}$; $\boldsymbol{P}$ is the vector of the electric polarization, $\{\sigma_{jk}\}$ the mechanical stress tensor. Here we see the combination of a second-rank tensor with a first-rank tensor.

Inverse Piezoelectric Tensor $\{\hat{d}_{ijk}\}$: $\varepsilon_{ij} = \hat{d}_{ijk}E_k$. The deformation $\{\varepsilon_{ij}\}$ proportional to the electric field strength is called first-order electrostriction. It is directly related to the piezoelectric effect.

First-Order Electrooptic Tensor $\{r_{ijk}\}$: $\Delta a_{ij} = r_{ijk}E_k$; $\{\Delta a_{ij}\}$ describes the change of the dielectric behavior in the optical region and thus $\{r_{ijk}\}$ the variation of the velocity of light as a function of the components of the electric field.

Nonohmic Conductivity $\{s_{ijk}\}$: $I_i = s_{ij}E_j + s_{ijk}E_jE_k$; the first term on the right describes the ohmic conductivity, the tensor $\{s_{ijk}\}$ the deviation from Ohm's law in quadratic dependence of the components of the electric field strength.

Hall Tensor $\{R_{ijk}\}$: $E_i = R_{ijk}I_jH_k$; the electric field strength generated by a current in the presence of a magnetic field is represented by a third-rank tensor.

Nonlinear Dielectric Tensor $\{\epsilon_{ijk}\}$: $D_i = \epsilon_{ij}E_j + \epsilon_{ijk}E_jE_k$; $\{\epsilon_{ijk}\}$ describes the deviation from linear behavior.

Fourth-Rank Tensors

I: Product of the coordinates of vectors (also mixed) and their differential quotients as well as the products of tensor components and corresponding differential quotients analogous to third-rank tensors e.g.,

$$\{x_ix_jx_kx_l\},\ \left\{\frac{\partial^4 F}{\partial x_i \partial x_j \partial x_k \partial x_l}\right\},\ \left\{\frac{\partial^2 F}{\partial t_{ij} \partial t_{kl}}\right\},\ \left\{\frac{\partial^3 E_i}{\partial x_j \partial x_k \partial x_l}\right\}.$$

II. *Elasticity Tensor* $\{c_{ijkl}\}$: $\sigma_{ij} = c_{ijkl}\varepsilon_{kl}$; there exists a linear combination of the components of the mechanical deformation tensor with the components of the mechanical stress tensor. The reversal is $\varepsilon_{ij} = s_{ijkl}\sigma_{kl}$. In static experiments, the second expression is mostly used and in dynamic experiments the first expression is favored.

Nonlinear Fourth-Rank Dielectric Tensors $\{\epsilon_{ijkl}\}$ and $\{f_{ijkl}\}$:

$$D_i = \epsilon_{ijkl}E_jE_kE_l \quad \text{or} \quad D_i = f_{ijkl}E_j\frac{\partial E_k}{\partial x_l}.$$

The first tensor describes, to a third-order approximation, the dielectric behavior in homogenous electric fields. The second tensor describes the dependence of products of the field strength and its variation (vector gradient).

Piezooptic and Photoelastic Tensors $\{p_{ijkl}\}$ and $\{q_{ijkl}\}$: $\Delta a_{ij} = q_{ijkl}\sigma_{kl}$ or $\Delta a_{ij} = p_{ijkl}\varepsilon_{kl}$; the change of the optical polarization constants Δa_{ij} under the influence of mechanical stresses or deformations is described to a first-order approximation by a fourth-rank tensor.

Second-Order Electrostriction $\{\hat{d}_{ijkl}\}$: $\varepsilon_{ij} = \hat{d}_{ijkl}E_kE_l$; this is the second-order approximation of electrostriction mentioned above.

Piezoelectric Effect by Electric Prepolarization $\{D_{ijkl}\}$: $P_i = D_{ijkl}E_j\sigma_{kl}$; electric polarization is generated by mechanical stress in the presence of an electric field.

Change in Magnetic Resistance $\{R_{ijkl}\}$: $E_i = R_{ijkl}I_jH_kH_l$; this is a property similar to the Hall effect, however, to second order of the components of the magnetic field strength.

Higher Rank Tensors

I: Products of tensor components and their differential quotients, especially those of mixed quantities.

II: *Second-Order Piezoelectric Effect* $\{d_{ijklm}\}$: $P_i = d_{ijklm}\sigma_{jk}\sigma_{lm}$; the second-order approximation of the piezoelectric effect is described by a fifth-rank tensor and the following approximations by tensors of odd rank.

Nonlinear Elasticity Tensor (Deviation from Hooke's law) $\{c_{ijklmn}\}$: for higher approximations, the relationship between deformation and stress is given by

$$\sigma_{ij} = c_{ijkl}\varepsilon_{kl} + c_{ijklmn}\varepsilon_{kl}\varepsilon_{mn} + c_{ijklmnop}\varepsilon_{kl}\varepsilon_{mn}\varepsilon_{op} + \cdots$$

Especially the easily observed nonlinear acoustic effects are reproduced with the help of sixth- and eighth-rank tensors.

Most higher tensor properties occur as higher approximations of simpler properties. Their tensorial representations follow analogous to the examples presented above.

3.7 Pseudo Tensors (Axial Tensors)

Our definition of tensors requires a supplement. Some quantities exist which only transform like normal tensor components when the coordinate system keeps its chirality (right- or left-handed system). We will explain this by considering the vector products $\boldsymbol{z} = \boldsymbol{x} \times \boldsymbol{y}$ of two position vectors $\boldsymbol{x}$ and $\boldsymbol{y}$ in the basic system. In the definition of the vector products, the handedness of the system spanned by three vectors $\boldsymbol{x}$, $\boldsymbol{y}$, and $\boldsymbol{x} \times \boldsymbol{y}$ is involved. Thus a change in the handedness of the reference system in a transformation must be taken into consideration. When applying a rotation–inversion operation $\boldsymbol{R}_{\bar{n}}$, which corresponds to the product of a normal rotation and an inversion, the right-handed reference system goes over into a left-handed system and vice versa. In the case of the inversion $\boldsymbol{R}_{\bar{1}}$, described by the transformation matrix

$$\boldsymbol{R}_{\bar{1}} = (u_{ij}) = \begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix},$$

we have $\boldsymbol{a}_i' = -\boldsymbol{a}_i$, $x_i' = -x_i$, and $y_i' = -y_i$. According to the prescription for calculating the vector product

$$\boldsymbol{z} = \boldsymbol{x} \times \boldsymbol{y} = V \begin{vmatrix} \boldsymbol{a}_1^* & \boldsymbol{a}_2^* & \boldsymbol{a}_3^* \\ x_1 & x_2 & x_3 \\ y_1 & y_2 & y_3 \end{vmatrix} = z_i \boldsymbol{a}_i^*$$

we also form, with the vectors $\boldsymbol{x}' = -x_i \boldsymbol{a}_i$ and $\boldsymbol{y}' = -y_i \boldsymbol{a}_i$, which results from the inversion of $\boldsymbol{x}$ and $\boldsymbol{y}$, the vector product and get $\boldsymbol{x}' \times \boldsymbol{y}' = \boldsymbol{z}$.

Thus $z_i' = z_i$ as opposed to $x_i' = -x_i$. According to this convention, the vector product produces a change in sign by an inversion compared to the transformation of a normal vector. The same applies to the case of an arbitrary rotation–inversion, as one can easily confirm. A change in sign does not occur with pure rotations. This special feature of the transformation of a vector, represented as the vector product of two normal vectors, is taken into consideration by multiplying the transformation formulae with the determinant $|u_{ij}|$ of the transformation matrix, which takes on the value $+1$ with a pure rotation, and the value -1 with a rotation–inversion.

Because of this difference to a normal vector, one designates the vector product of normal vectors as a *pseudo vector* or a first-rank *pseudo tensor*. Sometimes the designation "*axial vector*" is used contrary to a normal tensor, which is then termed "polar." This designation stems from the rotation vector $\boldsymbol{u}$, whose length specifies the rotation velocity or rotation angle and whose direction specifies the rotation axis, whereby the rotation is defined as clockwise, seen along the rotation vector.

Even with pseudo vectors of higher rank, which are always connected with first-rank tensors, a change in sign occurs with a change of handedness of the reference system, when the transformation formulae used so far are applied. The correct transformed quantities are also obtained when, in addition, the factor $|u_{ij}|$ is applied. For the transformation of pseudo tensors we then have

$$t'_{ij\ldots s} = |u_{ij}| u_{ii^*} u_{jj^*} \cdots u_{ss^*} t_{i^*j^*\ldots s^*}.$$

With the aid of a second-rank asymmetric tensor, where $t_{ij} = -t_{ji}$, we can represent the vector product $\boldsymbol{z} = \boldsymbol{x} \times \boldsymbol{y}$ by $z_i = t_{ij} y_j$. We assume the second-rank tensor written as a matrix:

$$(t_{ij}) = \begin{pmatrix} 0 & -x_3 & x_2 \\ x_3 & 0 & -x_1 \\ -x_2 & x_1 & 0 \end{pmatrix}.$$

When we perform an inversion in this representation of the vector product we get $z'_i = t'_{ij} y'_j = z_i$, where $t'_{ij} = -t_{ij}$ and thus the sign is different from $t'_{ij} = u_{ii^*} u_{jj^*} t_{i^*j^*}$. As a consequence, we can consider the vector product of two normal vectors (first-rank tensors) as a tensorial combination of a vector with a second-rank asymmetric pseudo tensor. The axial character of a tensor is propagated through the tensor operation. The following relationships derivable directly from the transformation behavior hold:

$$(p) = (p)(p), \quad (a) = (p)(a), \quad (a) = (a)(p), \quad (p) = (a)(a)$$

as well as further products derived from the above relationships. Here p and a are symbols for a polar (normal) and an axial tensor, respectively.

The most important group of pseudo tensors is associated with magnetic quantities. The vector of the magnetic field strength $\boldsymbol{H}$ and the vector of magnetic induction $\boldsymbol{B}$ are pseudo vectors.

One recognizes the axial character of $\boldsymbol{H}$ and $\boldsymbol{B}$ from Maxwell equations, the fundamental equations of electrodynamics. The equations are

$$\frac{1}{c}\frac{\partial \boldsymbol{D}}{\partial t} + I = \operatorname{rot} \boldsymbol{H},$$
$$\frac{1}{c}\frac{\partial \boldsymbol{B}}{\partial t} = -\operatorname{rot} \boldsymbol{E}.$$

where t is the time, $\boldsymbol{D}$, $\boldsymbol{I}$, and $\boldsymbol{E}$ are the vectors of electric displacement, current density, and electric field, and c the velocity of light; the symbol rot (read "rotation") represents the differential operator $\boldsymbol{\nabla}\times$, where $\boldsymbol{\nabla}$ signifies the differentiation vector $\boldsymbol{\nabla} = \frac{\partial}{\partial x_i}\boldsymbol{e}_i$, which we became acquainted with in the construction of gradients. In a Cartesian coordinate system, we have, for example,

$$\operatorname{rot}\boldsymbol{E} = \boldsymbol{\nabla}\times\boldsymbol{E} = \begin{vmatrix} \boldsymbol{e}_1 & \boldsymbol{e}_2 & \boldsymbol{e}_3 \\ \frac{\partial}{\partial x_1} & \frac{\partial}{\partial x_2} & \frac{\partial}{\partial x_3} \\ E_1 & E_2 & E_3 \end{vmatrix}$$

a pseudo vector (because of the vector product); on the other hand rot $\boldsymbol{H}$ is not a pseudo vector, because the axiality of $\boldsymbol{H}$ and rot compensate each other according to $(a)(a) = (p)$.

Further examples of pseudo tensors are the optical activity in the representation of the gyration tensor $\{\gamma_{ij}\}$, the scalar triple product of three vectors and the Levi-Cività symbol

$$e_{ijk} = \boldsymbol{e}_i \cdot (\boldsymbol{e}_j \times \boldsymbol{e}_k) \quad \text{with} \quad i,j,k = 1,2,3.$$

3.8 Symmetry Properties of Tensors

This section deals with the question of how far mathematical or physical arguments as well as symmetry properties of the crystals lead to relationships among the tensor components. In particular, we have to examine how these relationships reduce the number of independent tensor components.

3.8.1 Mathematical and Physical Arguments: Inherent Symmetry

Tensors often exhibit internal relationships among the index positions independent of the medium and its symmetry. For example, consider the so-called "symmetric" second-rank tensor whose components obey $t_{ij} = t_{ji}$ (six independent components). Each second-rank tensor can be decomposed into a symmetric part $t_{(ij)}$ and an antisymmetric part $t_{[ij]}$, according to

$$t_{ij} = \frac{t_{ij} + t_{ji}}{2} + \frac{t_{ij} - t_{ji}}{2} = t_{(ij)} + t_{[ji]}.$$

$t_{[ij]}$ has only three independent components.

Symmetric and antisymmetric tensors keep their symmetry character even with a change in the reference system, as can be easily checked. We previously pointed out the connection between the vector product and an antisymmetric second-rank tensor. In higher rank tensors, symmetric and antisymmetric

parts can be separated with respect to certain pairs of positions, as, for example, with a third-rank tensor

$$d_{ijk} = \frac{d_{ijk} + d_{ikj}}{2} + \frac{d_{ijk} - d_{ikj}}{2} = d_{i(jk)} + d_{i[jk]}.$$

A completely symmetric n-rank tensor exists when

$$t_{ij\ldots s} = t_{(ij\cdots s)},$$

where $(ij\ldots s)$ is an arbitrary permutation of the arrangement $ij\ldots s$. Such a tensor is termed total symmetric. An example is the tensor of the products of the coordinates of a vector $\boldsymbol{x}$ with the components

$$t_{ij\ldots s} = t_{(ij\ldots s)} = x_i x_j \cdots x_s = x_j x_i \cdots x_s = \cdots$$

and so on.

One can also define higher rank antisymmetric tensors in a similar manner. If, for example,

$$t_{ijk} = t_{[ijk]} = \frac{1}{3!}(t_{ijk} + t_{jki} + t_{kij} - t_{ikj} - t_{jik} - t_{kji}),$$

we are dealing with a fully antisymmetric tensor. As an example, we mention the Levi-Cività symbol $\{e_{ijk}\}$. This property is also conserved in each new reference system.

Apart from the permutation of indices within certain pairs of index positions, permutations of pairs or certain groups of pairs can also occur. As an example, we mention the elasticity tensor $\{c_{ijkl}\}$ with the property $c_{ijkl} = c_{(ij)(kl)} = c_{(kl)(ij)}$, i.e., the elasticity tensor is symmetric in the pairs of the 1 and 2 positions as well as the 3 and 4 positions, whereby the pairs are mutually permutable, too. An explanation will be given later.

Some quantities connected with the transport processes of charges, heat quantities or masses, for example, current densities and related properties such as magnetic fields, change their sense of direction when the time scale is reversed (time reversal). Accordingly, we distinguish between two groups:

- time invariant properties with $f(-t) = f(t)$, (t time) and
- non time invariant properties with $f(-t) = -f(t)$.

The generalization of these properties is such that one assigns, e.g., to each index position of a tensor a certain behavior with respect to time reversal. We will return to this point in Section 5.3.

3.8.2 Symmetry of the Medium

According to *Neumann's principle*, the property tensors must at least possess the symmetry group of the given crystal. This means that the tensor components must be invariant with respect to all symmetry operations of the given point symmetry group. In crystals, the only macroscopic symmetry operations that come into consideration are rotations $\boldsymbol{R}_n$ and rotation–inversions $\boldsymbol{R}_{\bar{n}}$.

For these special symmetry operations, the following relations must be fulfilled if they appear in the given point symmetry group:

$$t'_{ijk\ldots s} = u_{ii^*}u_{jj^*}\cdots u_{ss^*}t_{i^*j^*\ldots s^*} = t_{ij\ldots s}.$$

If h symmetry operations exist and if the maximum number of independent components is Z ($= n^m$ with an m-rank tensor in an n-dimensional space), then one gets a total of hZ such linear equations.

If h is the order of the symmetry group, the system of equations also contains the identity for each tensor component once, resulting in a total of $(h-1)Z$ nontrivial equations. In principle, it suffices only to apply the generators of the symmetry group. However, it is often useful to apply further symmetry operations such as, e.g., powers $\boldsymbol{R}_n^2$, $\boldsymbol{R}_n^3$, and so on, in order to simplify solving the system. If $h \geq 3$, the equations exhibit a strong linear dependence, often resulting in an enormous reduction in the number of independent components.

As a first example we consider the operation of an inversion center $\bar{1}$, whose transformation matrix is given by

$$\boldsymbol{R}_{\bar{1}} = \begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}.$$

As a result we have

$$t_{ij\ldots s} = (-1)^m t_{ij\ldots s}$$

because $u_{ii} = -1$ and $u_{ij} = 0$ for all $i \neq j$. This means that all odd-rank tensors completely vanish, when an inversion center exists. In particular, there exist no pyroelectric and piezoelectric effects. Furthermore, first-order electro-optical effects and the first-order nonlinear optical effects, as well as the deviation from first-order ohmic conductivity do not occur.

The situation is different with odd-rank pseudo tensors. They exist in the presence of $\bar{1}$ and the even-rank pseudo tensors vanish.

The inversion center has no influence on even-rank tensors. We can therefore say that these tensors are centro-symmetric, independent of the symmetry of the medium.

As a second example we consider the operation of a twofold axis parallel to $\boldsymbol{e}_1$ and a symmetry plane perpendicular to $\boldsymbol{e}_1$, represented as a rotation–inversion $\bar{2}$ parallel to $\boldsymbol{e}_1$. The associated transformation matrices are

$$\boldsymbol{R}_{2\|\boldsymbol{e}_1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix} \quad \text{and} \quad \boldsymbol{R}_{\bar{2}\|\boldsymbol{e}_1} = \begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

The transformation of the tensor components gives

$$t_{ij\ldots s} = (-1)^p t_{ij\ldots s} \quad \text{and} \quad t_{ij\ldots s} = (-1)^q t_{ij\ldots s}, \text{ respectively,}$$

where p stands for the number of the indices 2 and 3 and q for the number of the indices 1.

For p and q even we get the identity, i.e., these tensor components are not affected by the symmetry properties. The tensor components vanish for odd p and q. With even-rank tensors, if p is even or odd we also have q even or odd respectively. This means that even-rank tensors exhibit, in the case of a twofold axis or a mirror plane, the combined symmetry of a twofold axis and a symmetry plane perpendicular to this axis, in other words 2/m symmetry. With odd-rank tensors, the situation is different. If p is even, then q must be odd and vice versa because $p + q = m = 2r + 1$ (r integer). The components which vanish in the case of a twofold axis, exist in the case of a symmetry plane and vice versa. Thus the odd-rank tensors behave complementary with respect to the operation of a twofold axis or a symmetry plane. We will now consider, how large is the number of nonvanishing tensor components in both cases.

We first inquire for the number $Z_m(p)$ of components of an m-rank tensor possessing p times the index 1. For $p = 1$ we can choose the index 1 at m different positions. The other positions, namely $(m-1)$, can take on the index 2 or 3, thus having two degrees of freedom. This gives a total of $Z_1 = m \cdot 2^{(m-1)}$ tensor components with an index 1. We proceed in the same manner for $p > 1$. There exists m possibilities for the choice of the first index 1, for the second only $(m-1)$, for the third $(m-2)$, and so on. The number of these possibilities must, however, be divided by the number of nondistinguishable arrangements created, namely $p!$. The other index positions again have two degrees of freedom, so that a total of

$$Z_m(p) = \frac{m(m-1)(m-2)\cdots(m-p+1)}{p!} 2^{m-p} = \frac{m!}{p!(m-p)!} 2^{m-p}$$

components are concerned.

For the quotient we introduce the symbol $\binom{m}{p}$ used in combinatorial analysis. Thus the total number of tensor components possessing an odd number

of indices 1 is

$$Z'_m = \sum_{p'} \binom{m}{p'} 2^{(m-p')},$$

where p' runs through all odd numbers in the interval $1 \leq p' \leq m$.

Accordingly, one gets for the number of components where the index 1 appears an even number of times

$$Z''_m = \sum_{p''} \binom{m}{p''} 2^{(m-p'')} \text{ with } 0 \leq p'' \leq m; \quad p'' \text{ even.}$$

Since the index 1 occurs either an even or odd number of times in a component we have

$$Z'_m + Z''_m = Z = 3^m.$$

From this equation one finds for $m = 0, 1, 2, \ldots$:

$$Z'_m = (3^m - 1)/2 \text{ and hence also } Z''_m = (3^m + 1)/2.$$

If one investigates the operation of a twofold axis parallel to $\boldsymbol{e}_1$ or a symmetry plane perpendicular to $\boldsymbol{e}_1$ on a tensor in an n-dimensional space, where the transformation matrix is given by $u_{11} = 1$, $u_{ii} = -1$ for $i \neq 1$ and $u_{ij} = 0$ or $u_{11} = -1$, $u_{ii} = 1$ and $u_{ij} = 0$ $(i \neq j)$, respectively, one gets

$$Z'_m = \sum_{1 \leq p' \leq m} \binom{m}{p'} (n-1)^{(m-p')} = (n^m - (n-2)^m)/2$$

for the number with odd m and

$$Z''_m = (n^m + (n-2)^m)/2$$

for the number with even m. Our equations above are thus special cases for $n = 3$. The general validity of the equations for arbitrary m and n is easy to show with the help of a proof by induction when one substitutes

$$\binom{m+1}{p} = \binom{m}{p} + \binom{m}{p-1}$$

in the summation and checks the validity of the equation for $m = 0$ and 1 beforehand. We can now immediately specify the number of nonvanishing and independent tensor components Z_2 and $Z_{\bar{2}}$ when a twofold axis or symmetry plane is present. We have

$$Z_2 = Z_{\bar{2}} = (n^m + (n-2)^m)/2 \text{ for even } m,$$

however

$$Z_2 = (n^m - (n-2)^m)/2$$

and

$$Z_{\bar{2}} = (n^m + (n-2)^m)/2 \text{ for odd } m.$$

Now we include a second twofold axis parallel to $\boldsymbol{e}_2$ or a second symmetry plane perpendicular to $\boldsymbol{e}_2$. We then get for the point symmetry group 22 or $\bar{2}\bar{2}$=mm the number of nonvanishing independent components of tensors in a three-dimensional space

$$Z_{22} = Z_{\bar{2}\bar{2}} = (3^m + 3)/4 \text{ for even,}$$

however,

$$Z_{22} = (3^m - 3)/4 \text{ and } Z_{\bar{2}\bar{2}} = (3^m + 1)/4 \text{ for odd } m.$$

As proof we use the result for the number of components where one distinct index occurs an odd number of times, $Z' = (Z-1)/2$. If two indices should occur an odd number of times—here, the indices 1 and 2—then instead of Z one writes Z' and gets

$$(Z')' = (Z'-1)/2 = ((3^m-1)/2-1)/2 = (3^m-3)/4.$$

This is identical to the number of nonvanishing and independent components Z_{22} of an odd-rank tensor.

When two indices i and j are only allowed to occur an odd number of times, the third index must also occur an odd number of times. This means that Z_{22} and $Z_{\bar{2}\bar{2}}$ complement each other to $Z = n^m$ for odd m. For even m, all indices must occur an even number of times. Thus one must eliminate from the collection Z_2 those with an odd number of index 2, namely $Z' = (Z_2 - 1)/2$. This is accordingly $Z_{22} = Z_{\bar{2}\bar{2}} = Z_2 - Z' = (3^m + 3)/4$. Table 3.2 presents an overview of the number and type of independent tensor components for tensors up to rank 4.

For symmetry operations of three-, four- or sixfold rotation axes or rotation–inversion axes, the general relations are more complicated. We will treat these cases later in concrete examples. In all symmetry groups containing 2, $\bar{2}$, 22, or $\bar{2}\bar{2}$ as subgroups, the symmetry reduction is naturally only to be applied to tensor components existing in the respective subgroups. In Section 8.3 we will become acquainted with a group theoretical method to calculate the number and type of independent tensor components for arbitrary symmetry groups.

Table 3.2 Independent and non-vanishing tensor components for the cases of a twofold axis (2) parallel to $\boldsymbol{e}_1$, a mirror plane ($\bar{2}$) perpendicular to $\boldsymbol{e}_1$, two twofold axes (22) parallel to $\boldsymbol{e}_1$ and $\boldsymbol{e}_2$ and two mirror planes ($\bar{2}\bar{2} =$ mm) perpendicular to $\boldsymbol{e}_1$ and $\boldsymbol{e}_2$. The number of independent tensor components is given in parentheses.

Conditions for existing $t_{ij\ldots s}$:
a) 2 or $\bar{2}$ parallel $\boldsymbol{e}_k$, m even: index k even times.
b) 2 parallel $\boldsymbol{e}_k$, m odd: index k odd times.
c) $\bar{2}$ parallel $\boldsymbol{e}_k$, m odd: index k odd times.
d) 22 or $\bar{2}\bar{2}$ parallel $\boldsymbol{e}_k$ and $\boldsymbol{e}_l$, m even: indices k and l even times.
e) 22 parallel $\boldsymbol{e}_i$, m odd: all indices even times.
f) $\bar{2}\bar{2}$ parallel $\boldsymbol{e}_k$ and $\boldsymbol{e}_l$, m odd: indices k and l even times.

	$2 \parallel \boldsymbol{e}_1$	$\bar{2} \parallel \boldsymbol{e}_1$	$22 \parallel \boldsymbol{e}_1$ and $\boldsymbol{e}_2$	$\bar{2}\bar{2} \parallel \boldsymbol{e}_1$ and $\boldsymbol{e}_2$
Z_m, m even	$(3^m+1)/2$	$(3^m+1)/2$	$(3^m+3)/4$	$(3^m+3)/4$
Z_m, m odd	$(3^m-1)/2$	$(3^m+1)/2$	$(3^m-3)/4$	$(3^m+1)/4$
$m=0$	t (1)	t (1)	t (1)	t (1)
$m=1$	t_1 (1)	t_2, t_3 (2)	(0)	t_3 (1)
$m=2$	$t_{11}, t_{22}, t_{33}, t_{23}, t_{32}$ (5)	$t_{11}, t_{22}, t_{33}, t_{23}, t_{32}$ (5)	t_{11}, t_{22}, t_{33} (3)	t_{11}, t_{22}, t_{33} (3)
$m=3$	$t_{123}, t_{132}, t_{231}, t_{213}, t_{312}, t_{321}, t_{122}, t_{212}, t_{221}, t_{133}, t_{313}, t_{331}, t_{111}$ (13)	$t_{112}, t_{121}, t_{211}, t_{113}, t_{131}, t_{311}, t_{223}, t_{232}, t_{322}, t_{332}, t_{323}, t_{233}, t_{222}, t_{333}$ (14)	$t_{123}, t_{132}, t_{231}, t_{213}, t_{312}, t_{321}$ (6)	$t_{113}, t_{131}, t_{311}, t_{223}, t_{232}, t_{322}, t_{333}$ (7)
$m=4$	$t_{1111}, t_{1122}, t_{1133}, t_{2211}, t_{3311}, t_{1123}, t_{1132}, t_{2311}, t_{3211}, t_{1213}, t_{1321}, t_{1231}, t_{1321}, t_{2131}, t_{3121}, t_{2311}, t_{3211}, t_{1212}, t_{1221}, t_{2112}, t_{2121}, t_{1313}, t_{1331}, t_{3113}, t_{3131}, t_{2222}, t_{2233}, t_{3322}, t_{2223}, t_{2232}, t_{2322}, t_{3222}, t_{2323}, t_{2332}, t_{3223}, t_{3232}, t_{3333}, t_{3332}, t_{3323}, t_{3233}, t_{2333}$ (41)	$t_{1111}, t_{1122}, t_{1133}, t_{2211}, t_{3311}, t_{1123}, t_{1132}, t_{2311}, t_{3211}, t_{1213}, t_{1321}, t_{1231}, t_{1321}, t_{2131}, t_{3121}, t_{2311}, t_{3211}, t_{1212}, t_{1221}, t_{2112}, t_{2121}, t_{1313}, t_{1331}, t_{3113}, t_{3131}, t_{2222}, t_{2233}, t_{3322}, t_{2223}, t_{2232}, t_{2322}, t_{3222}, t_{2323}, t_{2332}, t_{3223}, t_{3232}, t_{3333}, t_{3332}, t_{3323}, t_{3233}, t_{2333}$ (41)	$t_{1111}, t_{1122}, t_{2211}, t_{1212}, t_{1221}, t_{2121}, t_{2112}, t_{1133}, t_{3311}, t_{1313}, t_{1331}, t_{3113}, t_{3131}, t_{2222}, t_{2233}, t_{3322}, t_{2323}, t_{2332}, t_{3223}, t_{3232}, t_{333}$ (21)	$t_{1111}, t_{1122}, t_{2211}, t_{1212}, t_{1221}, t_{2121}, t_{2112}, t_{1133}, t_{3311}, t_{1313}, t_{1331}, t_{3113}, t_{3131}, t_{2222}, t_{2233}, t_{3322}, t_{2323}, t_{2332}, t_{3223}, t_{3232}, t_{333}$ (21)

$\bar{2}$ parallel $\boldsymbol{e}_1$ signifies a mirror plane perpendicular to $\boldsymbol{e}_1$.

3.9 Derived Tensors and Tensor Invariants

Through the operation of multiplication and tensor contraction with itself as well as with nonspecific tensors, such as the tensors of the Kronecker symbol (spherical tensor), the Levi-Cività tensor, the position vector, and their combinations, one obtains, according to the rules just discussed, new tensors that are often more accessible to an interpretation than the given initial tensor.

The group of tensor powers comes into play, with respect to the generating quantities, in higher order effects, e.g., the tensor $\{E_i E_j\}$ of the components of the electric field strength. For an m-rank tensor, the *quadric tensor* is

$$t^2_{ij\ldots s,i^*j^*\ldots s^*} = t_{ij\ldots s} t_{i^*j^*\ldots s^*}$$

a $2m$-rank tensor. In an analogous manner, one can form the *zth power* of a tensor

$$t_{ij\ldots s,i^*j^*\ldots s^*,i^{**}j^{**}\ldots s^{**}\ldots} = t_{ij\ldots s} t_{i^*j^*\ldots s^*} t_{i^{**}j^{**}\ldots s^{**}\ldots}.$$

In self-contraction, one deals with the generation of tensors of the type

$$t_{ij\ldots ri^*j^*\ldots r^*} = t_{ij\ldots rs} t_{i^*j^*\ldots r^*s} \quad \text{contraction over the } m\text{th position (index } s\text{)}.$$

Multiple contractions can also occur, whereby the indices, over which are to be summed, can take on different positions. Of importance is the complete contraction over all positions

$$Q = t_{ij\ldots s} t_{ij\ldots s},$$

a scalar invariant, independent of the reference system. In the case of a vector $\boldsymbol{x}$, Q corresponds to the square of the magnitude (length) of the vector $Q = x_i x_i = x_1^2 + x_2^2 + x_3^2$. Accordingly, Q can in general be designated as the square of the magnitude of a tensor. With respect to the contraction with other tensors, special emphasis is paid to the total contraction with tensors of the corresponding products of the components of the position vector:

$$F = t_{ij\ldots s} x_i x_j \cdots x_s.$$

This expression represents for a fixed F a surface of mth order, the so-called *tensor surface*. If one inserts, instead of $t_{ij\ldots s}$, the components of the associated total symmetric tensor, one gets the same tensor surface. This means that the tensor surface reproduces the complete tensor properties only in the case of a total symmetric tensor. The tensor surface allows one to represent one of the most important tensor properties, the so-called *longitudinal effect*, in a quite instructive manner as we shall see in the next section.

Further interesting contractions can be generated with the help of the tensors of the Kronecker symbol $\delta_{ij} = 1$ for $i = j$ and $= 0$ for $i \neq j$ or the Levi-Cività symbol $e_{ijk} = \boldsymbol{e}_i \cdot (\boldsymbol{e}_j \times \boldsymbol{e}_k)$. As an example, we mention the scalar invariants for even-rank tensors

$$I = t_{ijkl\ldots rs} \delta_{ij} \delta_{kl} \cdots \delta_{rs}.$$

The operation $t_{ij\ldots s}\delta_{im} = t_{mj\ldots s}$ exchanges an index. This can be carried out any number of times. Important contraction types for fourth-rank tensors are

$$A_{jl} = t_{ijkl}\delta_{ik}, \quad B_{kl} = t_{ijkl}\delta_{ij}, \quad C_{ik} = t_{ijkl}\delta_{jl}, \quad \text{and} \quad D_{ij} = t_{ijkl}\delta_{kl};$$

here we are dealing with second-rank tensor invariants arising from fourth-rank tensors.

As an example of the application of the Levi-Cività symbol, we consider the vector $\boldsymbol{q}$ (pseudo vector), assigned to a second-rank tensor, possessing the components $q_k = t_{ij}e_{ijk}$ as well as the vector product of the vectors $\boldsymbol{x}$ and $\boldsymbol{y}$, namely $\boldsymbol{z} = \boldsymbol{x} \times \boldsymbol{y}$, that can also be represented by $z_k = x_i y_i e_{ijk}$ in a Cartesian reference system. The triple vector product of $\boldsymbol{x}$, $\boldsymbol{y}$, and $\boldsymbol{z}$ gives $\boldsymbol{x} \cdot (\boldsymbol{y} \times \boldsymbol{z}) = x_i y_i z_k e_{ijk}$, an invariant representation in any Cartesian reference system.

Furthermore, we should mention invariants derived from fourth-rank tensors

$$S_{mn} = t_{ijkl}e_{ijm}e_{kln} \quad \text{and} \quad T_{mn} = t_{ijkl}e_{ikm}e_{jln}$$

as well as similar operations, which in part, are of practical importance.

Other examples will be treated in our discussion of concrete properties. Here we want to emphasize the special importance of scalar invariants because they indicate a directionally independent value, which can normally be interpreted as a spatial mean value of a certain tensor property.

At this point we must forgo a systematic discussion of invariants, although just now a number of very fascinating problems emerge, e.g., the question of the number of independent variables of a tensor, the decomposition and construction of a tensor with a basis of invariants. Naturally, we can safely answer the first question by saying that the number of independent invariants cannot be larger than the number of independent tensor components. Useful aids in the discussion of such relationships are available from group theory, which we shall return to in a later section.

3.10 Longitudinal and Transverse Effects

If two vectors $\boldsymbol{A}$ and $\boldsymbol{B}$ are connected via a second-rank tensor according to $B_i = t_{ij}A_j$, then both vectors run parallel only in distinct directions. For arbitrary directions of $\boldsymbol{A}$ we can analyze the decomposition of $\boldsymbol{B}$ into components parallel and perpendicular to $\boldsymbol{A}$. We get

$$\boldsymbol{B}_{\|\boldsymbol{A}} = B_i A_i \boldsymbol{A}/A^2 = t_{ij}A_i A_j \boldsymbol{A}/A^2.$$

We specify the unit vector in the direction of $\boldsymbol{A}$ by $\boldsymbol{e}'_1 = \boldsymbol{A}/A = u_{1i}\boldsymbol{e}_i$. We then get

$$\boldsymbol{B}_{\|\boldsymbol{A}} = u_{1i}u_{1j}t_{ij}\boldsymbol{A}.$$

We call the quantity $u_{1i}u_{1j}t_{ij} = t'_{11}$ the longitudinal effect of the given tensor property. It describes, e.g., in the case of electrical conductivity, the conductivity in the direction of the electric field strength. We now emphasize that this

longitudinal effect is normally easily amenable to measurements. By transformation, it can be immediately calculated for any direction. Correspondingly, there exists a transverse effect for a component of $\boldsymbol{B}$ perpendicular to $\boldsymbol{A}$ in the direction $\boldsymbol{e}'_2$, which can be arbitrarily chosen to be perpendicular to $\boldsymbol{e}'_1$. We get the quantity t'_{21}, in which the vector $\boldsymbol{A}$ as the generating quantity parallel to $\boldsymbol{e}'_1$ and the part $\boldsymbol{B}$ parallel to $\boldsymbol{e}'_2$ are connected to each other. We call $t'_{21} = u_{2i}u_{1j}t_{ij}$ the transverse effect in the direction $\boldsymbol{e}'_2$ by excitation in the direction $\boldsymbol{e}'_1$.

The general definition of longitudinal and transverse effects looks like this: We consider the longitudinal component $A'_{111\ldots1}$ of a generating quantity in the direction $\boldsymbol{e}'_1$ and observe the associated longitudinal component of the generated quantity $B'_{111\ldots1}$ or the component $B'_{222\ldots2}$ in the direction $\boldsymbol{e}'_1$ or $\boldsymbol{e}'_2$, respectively.

In the operation $B'_{111\ldots1} = t'_{111\ldots1}A'_{111\ldots1}$, $t'_{111\ldots1} = u_{1i}u_{1j}\cdots u_{1s}t_{ij\ldots s}$ is the longitudinal component for the direction $\boldsymbol{e}'_1 = u_{1i}\boldsymbol{e}_i$, and in $B'_{222\ldots2} = t'_{222\ldots2111\ldots1}A'_{111\ldots1}$, $t'_{222\ldots2111\ldots1}$ is the transverse component for the direction $\boldsymbol{e}'_2 = u_{2i}\boldsymbol{e}_i$ by excitation in the direction $\boldsymbol{e}'_1 = u_{1i}\boldsymbol{e}_i$. Although there exists only one longitudinal effect for a direction $\boldsymbol{e}'_1$, one can calculate transverse effects in directions perpendicular to $\boldsymbol{e}'_1$.

An interesting relation exists between the tensor surface and the longitudinal effect. We consider a direction along the position vector $\boldsymbol{x} = x_i\boldsymbol{e}_i = |\boldsymbol{x}|\boldsymbol{e}'_1$. Here, $\boldsymbol{e}'_1 = u_{1i}\boldsymbol{e}_i$ with $u_{1i} = x_i|\boldsymbol{x}|^{-1}$. Thus for the longitudinal component of an m-rank tensor we get

$$t'_{111\ldots1} = u_{1i}u_{1j}\ldots u_{1s}t_{ij\ldots s} = x_ix_j\ldots x_st_{ij\ldots s}|\boldsymbol{x}|^{-m}.$$

We substitute the numerator of the quotient by $F = x_ix_j\cdots x_st_{ij\ldots s}$, the scalar invariant of the tensor surface, and get $t'_{111\ldots1} = F|\boldsymbol{x}|^{-m}$. This means that the longitudinal component in the direction $\boldsymbol{x}$ is equal to F divided by the mth power of the distance of the end point of $\boldsymbol{x}$ on the tensor surface from the origin of the reference system. Thus the tensor surface gains an intuitive physical meaning.