

1.2. General introduction to the subgroups of space groups

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1.2.1. General remarks

The performance of simple vector and matrix calculations, as well as elementary operations with groups, are nowadays common practice in crystallography, especially since computers and suitable programs have become widely available. The authors of this volume therefore assume that the reader has at least some practical experience with matrices and groups and their crystallographic applications. The explanations and definitions of the basic terms of linear algebra and group theory in these first sections of this introduction are accordingly short. Rather than replace an elementary textbook, these first sections aim to acquaint the reader with the method of presentation and the terminology that the authors have chosen for the tables and graphs of this volume. The concepts of groups, their subgroups, isomorphism, coset decomposition and conjugacy are considered to be essential for the use of the tables and for their practical application to crystal structures; for a deeper understanding the concept of normalizers is also necessary. Frequently, however, an ‘intuitive feeling’ obtained by practical experience may replace a full comprehension of the mathematical meaning. From Section 1.2.6 onwards, the presentation will be more detailed because the subjects are more specialized (but mostly not more difficult) and are seldom found in textbooks.

1.2.2. Mappings and matrices

1.2.2.1. Crystallographic symmetry operations

A crystal is a finite block of an infinite periodic array of atoms in physical space. The infinite periodic array is called the *crystal pattern*. The finite block is called the *macroscopic crystal*.

Periodicity implies that there are *translations* which map the crystal pattern onto itself. Geometric mappings have the property that for each point P of the space, and thus of the object, there is a uniquely determined point \tilde{P} , the *image point*. The mapping is *reversible* if each image point \tilde{P} is the image of one point P only.

Translations belong to a special category of mappings which leave all distances in the space invariant (and thus within an object and between objects in the space). Furthermore, a mapping of an object onto itself (German: *Deckoperation*) is the basis of the concept of geometric symmetry. This is expressed by the following two definitions.

Definition 1.2.2.1.1. A mapping is called a *motion*, a *rigid motion* or an *isometry* if it leaves all distances invariant (and thus all angles, as well as the size and shape of an object). In this volume the term ‘isometry’ is used. \square

An isometry is a special kind of affine mapping. In an *affine mapping*, parallel lines are mapped onto parallel lines; lengths and angles may be distorted but quotients of lengths on the same line are preserved. In Section 1.2.2.3, the description of affine mappings is discussed, because this type of description also applies to isometries. Affine mappings are important for the classification of crystallographic symmetries, cf. Section 1.2.5.2.

Definition 1.2.2.1.2. A mapping is called a *symmetry operation* of an object if

- (1) it is an isometry,
- (2) it maps the object onto itself. \square

Instead of ‘maps the object onto itself’, one frequently says ‘leaves the object invariant (as a whole)’. This does not mean that each point of the object is mapped onto itself; rather, the object is mapped in such a way that an observer cannot distinguish the states of the object before and after the mapping.

Definition 1.2.2.1.3. A symmetry operation of a crystal pattern is called a *crystallographic symmetry operation*. \square

The symmetry operations of a macroscopic crystal are also crystallographic symmetry operations, but they belong to another kind of mapping which will be discussed in Section 1.2.5.4.

There are different types of isometries which may be crystallographic symmetry operations. These types are described and discussed in many textbooks of crystallography and in mathematical, physical and chemical textbooks. They are listed here without further treatment. Fixed points are very important for the characterization of isometries.

Definition 1.2.2.1.4. A point P is a *fixed point* of a mapping if it is mapped onto itself, i.e. the *image point* \tilde{P} is the same as the original point P : $\tilde{P} = P$. \square

The set of all fixed points of an isometry may be the whole space, a plane in the space, a straight line, a point, or the set may be empty (no fixed point).

The following kinds of isometries exist:

- (1) The *identity operation*, which maps each point of the space onto itself. It is a symmetry operation of every object and, although trivial, is indispensable for the group properties which are discussed in Section 1.2.3.
- (2) A *translation* t which shifts every object. A translation is characterized by its translation vector \mathbf{t} and has no fixed point: if \mathbf{x} is the column of coordinates of a point P , then the coordinates $\tilde{\mathbf{x}}$ of the image point \tilde{P} are $\tilde{\mathbf{x}} = \mathbf{x} + \mathbf{t}$. If a translation is a symmetry operation of an object, the object extends infinitely in the directions of \mathbf{t} and $-\mathbf{t}$. A translation preserves the ‘handedness’ of an object, e.g. it maps any right-hand glove onto a right-hand one and any left-hand glove onto a left-hand one.
- (3) A *rotation* is an isometry that leaves one line fixed pointwise. This line is called the *rotation axis*. The degree of rotation about this axis is described by its rotation angle φ . In particular, a rotation is called an *N -fold rotation* if the rotation angle is $\varphi = k \times 360^\circ / N$, where k and N are relatively prime integers. A rotation preserves the ‘handedness’ of any object.
- (4) A *screw rotation* is a rotation coupled with a translation parallel to the rotation axis. The rotation axis is now called the *screw axis*. The translation vector is called the *screw vector*. A screw rotation has no fixed points. The screw axis is invariant as a whole under the screw rotation but not pointwise.
- (5) An *N -fold rotoinversion* is an *N -fold rotation* coupled with inversion through a point on the rotation axis. This point is called the *centre of the rotoinversion*. For $N \neq 2$ it is the only fixed point. The axis of the rotation is invariant as a whole

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under the rotoinversion and is called its *rotoinversion axis*. A rotoinversion changes the handedness by its inversion component: it maps any right-hand glove onto a left-hand one and *vice versa*. Performed twice it results in a rotation. Special rotoinversions are those for $N = 1$ and $N = 2$, which are dealt with separately.

- (6) The *inversion* can be considered as a onefold rotoinversion ($N = 1$). The fixed point is called the *inversion centre* or the *centre of symmetry*.
- (7) A twofold rotoinversion ($N = 2$) is called a *reflection* or a *reflection through a plane*. It is an isometry which leaves a plane perpendicular to the twofold rotoinversion axis fixed pointwise. This plane is called the *reflection plane* or *mirror plane* and it intersects the rotation axis in the centre of the rotoinversion. Its orientation is described by the direction of its normal vector, *i.e.* of the rotation axis. For a twofold rotoinversion, neither the rotation nor the inversion are symmetry operations themselves. As for any other rotoinversion, the reflection changes the handedness of an object.
- (8) A *glide reflection* is a reflection through a plane coupled with a translation parallel to this plane. The translation vector is called the *glide vector*. A glide reflection changes the handedness and has no fixed point. The former reflection plane is now called the *glide plane*. Under a glide reflection, the glide plane is invariant as a whole but not pointwise.

Symmetry operations of crystal patterns may belong to any of these isometries. The set of all symmetry operations of a crystal pattern has the following properties: performing two (and thus more) symmetry operations one after the other results in another symmetry operation. Moreover, there is the identity operation in this set, *i.e.* an operation that leaves every point of the space and thus of the crystal pattern fixed. Finally, for any symmetry operation of an object there is an ‘inverse’ symmetry operation by which its effect is reversed. These properties are necessary for the application of group theory, *cf.* Section 1.2.3.

1.2.2.2. Coordinate systems and coordinates

To describe mappings analytically, one introduces a coordinate system $\{O, \mathbf{a}, \mathbf{b}, \mathbf{c}\}$, consisting of three linearly independent (*i.e.* not coplanar) basis vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}$ (or $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$) and an origin O . For the plane (two-dimensional space) an origin and two linearly independent (*i.e.* not parallel) basis vectors \mathbf{a}, \mathbf{b} (or $\mathbf{a}_1, \mathbf{a}_2$) are chosen. Referred to this coordinate system, each point P can be described by three (or two for the plane) coordinates x, y, z (or x_1, x_2, x_3). An object, *e.g.* a crystal, can now be described by a continuous or discontinuous function of the coordinates such as the electron density or the coordinates of the centres of the atoms. A mapping can be regarded as an instruction of how to calculate the coordinates $\tilde{x}, \tilde{y}, \tilde{z}$ of the image point \tilde{X} from the coordinates x, y, z of the original point X .

In contrast to the practice in physics and chemistry, a non-Cartesian coordinate system is usually chosen in crystallography. The primary aim of the choice of the crystallographic coordinate system is to describe the crystal pattern and its set of all symmetry operations in a simple way. This aim holds in particular for the infinitely many symmetry translations of the crystal pattern, which form its *translation group*. Secondary to this aim are equality of the lengths of, and right angles between, the basis vectors.

The vector \mathbf{t} belonging to the translation t is called a *translation vector* or a *lattice vector*. The set of all translation vectors of the crystal pattern is called its *vector lattice* \mathbf{L} . Both the transla-

tion group and the vector lattice are useful tools for describing the periodicity of the crystals.

For the description of a vector lattice several kinds of bases are in use. Orthonormal bases are not the most convenient, because the coefficients of the lattice vectors may then be any real number. The coefficients of the lattice vectors are more transparent if the basis vectors themselves are lattice vectors.

Definition 1.2.2.2.1. A basis which consists of lattice vectors of a crystal pattern is called a *lattice basis* or a *crystallographic basis*. \square

Referred to a lattice basis, each lattice vector $\mathbf{t} \in \mathbf{L}$ is a linear combination of the basis vectors with *rational coefficients*. One can even select special bases such that the coefficients of all lattice vectors are integers.

Definition 1.2.2.2.2. A crystallographic basis is called a *primitive basis* if every lattice vector has integer coefficients. \square

A fundamental feature of vector lattices is that for any lattice in a dimension greater than one an infinite number of primitive bases exists. With certain rules, the choice of a primitive basis can be made unique (reduced bases). In practice, however, the *conventional bases* are not always primitive; the choice of a conventional basis is determined by the matrix parts of the symmetry operations, *cf.* Section 1.2.5.1.

1.2.2.3. The description of mappings

The instruction for the calculation of the coordinates of \tilde{X} from the coordinates of X is simple for an affine mapping and thus for an isometry. The equations are

$$\begin{aligned}\tilde{x} &= W_{11}x + W_{12}y + W_{13}z + w_1 \\ \tilde{y} &= W_{21}x + W_{22}y + W_{23}z + w_2 \\ \tilde{z} &= W_{31}x + W_{32}y + W_{33}z + w_3,\end{aligned}\tag{1.2.2.1}$$

where the coefficients W_{ik} and w_j are constant. These equations can be written using the matrix formalism:

$$\begin{pmatrix} \tilde{x} \\ \tilde{y} \\ \tilde{z} \end{pmatrix} = \begin{pmatrix} W_{11} & W_{12} & W_{13} \\ W_{21} & W_{22} & W_{23} \\ W_{31} & W_{32} & W_{33} \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{pmatrix} w_1 \\ w_2 \\ w_3 \end{pmatrix}.\tag{1.2.2.2}$$

This matrix equation is usually abbreviated by

$$\tilde{\mathbf{x}} = \mathbf{W}\mathbf{x} + \mathbf{w},\tag{1.2.2.3}$$

where

$$\tilde{\mathbf{x}} = \begin{pmatrix} \tilde{x} \\ \tilde{y} \\ \tilde{z} \end{pmatrix}, \mathbf{x} = \begin{pmatrix} x \\ y \\ z \end{pmatrix}, \mathbf{w} = \begin{pmatrix} w_1 \\ w_2 \\ w_3 \end{pmatrix} \text{ and } \mathbf{W} = \begin{pmatrix} W_{11} & W_{12} & W_{13} \\ W_{21} & W_{22} & W_{23} \\ W_{31} & W_{32} & W_{33} \end{pmatrix}.$$

Definition 1.2.2.3.1. The matrix \mathbf{W} is called the *linear part* or *matrix part*, the column \mathbf{w} is the *translation part* or *column part* of a mapping. \square

In equations (1.2.2.1) and (1.2.2.3), the coordinates are mixed with the quantities describing the mapping, designated by the letters W_{ik} and w_j or \mathbf{W} and \mathbf{w} . Therefore, one prefers to write equation (1.2.2.3) in the form

$$\tilde{\mathbf{x}} = (\mathbf{W}, \mathbf{w})\mathbf{x} \text{ or } \tilde{\mathbf{x}} = \{\mathbf{W} | \mathbf{w}\}\mathbf{x}.\tag{1.2.2.4}$$

The symbols (\mathbf{W}, \mathbf{w}) and $\{\mathbf{W} | \mathbf{w}\}$ which describe the mapping referred to the chosen coordinate system are called the *matrix-column pair* and the *Seitz symbol*.

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The formulae for the combination of affine mappings and for the inverse of an affine mapping (regular matrix \mathbf{W}) are obtained by

$$\begin{aligned}\tilde{\mathbf{x}} &= \mathbf{W}_1 \mathbf{x} + \mathbf{w}_1, \quad \tilde{\tilde{\mathbf{x}}} = \mathbf{W}_2 \tilde{\mathbf{x}} + \mathbf{w}_2 = \mathbf{W}_3 \mathbf{x} + \mathbf{w}_3 \\ \tilde{\tilde{\mathbf{x}}} &= \mathbf{W}_2 (\mathbf{W}_1 \mathbf{x} + \mathbf{w}_1) + \mathbf{w}_2 = \mathbf{W}_2 \mathbf{W}_1 \mathbf{x} + \mathbf{W}_2 \mathbf{w}_1 + \mathbf{w}_2.\end{aligned}$$

From $\tilde{\mathbf{x}} = \mathbf{W}\mathbf{x} + \mathbf{w}$, it follows that $\mathbf{W}^{-1}\tilde{\mathbf{x}} = \mathbf{x} + \mathbf{W}^{-1}\mathbf{w}$ or $\mathbf{x} = \mathbf{W}^{-1}\tilde{\mathbf{x}} - \mathbf{W}^{-1}\mathbf{w}$.

Using matrix–column pairs, this reads

$$(\mathbf{W}_3, \mathbf{w}_3) = (\mathbf{W}_2, \mathbf{w}_2) (\mathbf{W}_1, \mathbf{w}_1) = (\mathbf{W}_2 \mathbf{W}_1, \mathbf{W}_2 \mathbf{w}_1 + \mathbf{w}_2) \quad (1.2.2.5)$$

and

$$\mathbf{x} = (\mathbf{W}, \mathbf{w})^{-1} \tilde{\mathbf{x}} = (\mathbf{W}', \mathbf{w}') \tilde{\mathbf{x}}$$

or

$$(\mathbf{W}', \mathbf{w}') = (\mathbf{W}, \mathbf{w})^{-1} = (\mathbf{W}^{-1}, -\mathbf{W}^{-1}\mathbf{w}). \quad (1.2.2.6)$$

One finds from equations (1.2.2.5) and (1.2.2.6) that the linear parts of the matrix–column pairs transform as one would expect:

- (1) the linear part of the product of two matrix–column pairs is the product of the linear parts, *i.e.* if $(\mathbf{W}_3, \mathbf{w}_3) = (\mathbf{W}_2, \mathbf{w}_2) (\mathbf{W}_1, \mathbf{w}_1)$ then $\mathbf{W}_3 = \mathbf{W}_2 \mathbf{W}_1$;
- (2) the linear part of the inverse of a matrix–column pair is the inverse of the linear part, *i.e.* if $(\mathbf{X}, \mathbf{x}) = (\mathbf{W}, \mathbf{w})^{-1}$, then $\mathbf{X} = \mathbf{W}^{-1}$. [This relation is included in the first one: from $(\mathbf{W}, \mathbf{w})(\mathbf{X}, \mathbf{x}) = (\mathbf{W}\mathbf{X}, \mathbf{W}\mathbf{x} + \mathbf{w}) = (\mathbf{I}, \mathbf{o})$ follows $\mathbf{X} = \mathbf{W}^{-1}$. Here \mathbf{I} is the unit matrix and \mathbf{o} is the column consisting of zeroes].

These relations will be used in Section 1.2.5.4.

For the column parts, equations (1.2.2.5) and (1.2.2.6) are less convenient:

$$(1) \mathbf{w}_3 = \mathbf{W}_2 \mathbf{w}_1 + \mathbf{w}_2; \quad (2) \mathbf{w}' = -\mathbf{W}^{-1}\mathbf{w}.$$

Because of the inconvenience of these relations, it is often preferable to use ‘augmented’ matrices, by which one can describe the combination of affine mappings and the inverse mapping by the equations of the usual matrix multiplication. These matrices are introduced in the next section.

1.2.2.4. Matrix–column pairs and $(n+1) \times (n+1)$ matrices

It is natural to combine the matrix part and the column part describing an affine mapping to form a (3×4) matrix, but such matrices cannot be multiplied by the usual matrix multiplication and cannot be inverted. However, if one supplements the (3×4) matrix by a fourth row ‘0 0 0 1’, one obtains a (4×4) square matrix which can be combined with the analogous matrices of other mappings and can be inverted. These matrices are called *augmented matrices* and are designated by open-face letters in this volume:

$$\mathbb{W} = \left(\begin{array}{ccc|c} \mathbf{W}_{11} & \mathbf{W}_{12} & \mathbf{W}_{13} & \mathbf{w}_1 \\ \mathbf{W}_{21} & \mathbf{W}_{22} & \mathbf{W}_{23} & \mathbf{w}_2 \\ \mathbf{W}_{31} & \mathbf{W}_{32} & \mathbf{W}_{33} & \mathbf{w}_3 \\ \hline 0 & 0 & 0 & 1 \end{array} \right), \quad \tilde{\mathbf{x}} = \begin{pmatrix} \tilde{x} \\ \tilde{y} \\ \tilde{z} \\ 1 \end{pmatrix}, \quad \mathbf{x} = \begin{pmatrix} x \\ y \\ z \\ 1 \end{pmatrix}. \quad (1.2.2.7)$$

In order to write equation (1.2.2.3) as $\tilde{\mathbf{x}} = \mathbb{W}\mathbf{x}$ with the augmented matrices \mathbb{W} , the columns $\tilde{\mathbf{x}}$ and \mathbf{x} also have to be extended to the augmented columns $\tilde{\mathbf{x}}$ and \mathbf{x} . Equations (1.2.2.5) and (1.2.2.6) then become

$$\mathbb{W}_3 = \mathbb{W}_2 \mathbb{W}_1 \quad \text{and} \quad (\mathbb{W})^{-1} = (\mathbb{W}^{-1}). \quad (1.2.2.8)$$

The vertical and horizontal lines in the matrix have no mathematical meaning. They are simply a convenience for separating the matrix part from the column part and from the row ‘0 0 0 1’, and could be omitted.

Augmented matrices are very useful when writing down general formulae which then become more transparent and more elegant. However, the matrix–column pair formalism is, in general, advantageous for practical calculations.

For the augmented columns of vector coefficients, see Section 1.2.2.6.

1.2.2.5. Isometries

Isometries are special affine mappings, as in Definition 1.2.2.1.1. The matrix \mathbf{W} of an isometry has to fulfil conditions which depend on the coordinate basis. These conditions are:

- (1) A basis $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ is characterized by the scalar products $(\mathbf{a}_j, \mathbf{a}_k)$ of its basis vectors or by its *lattice parameters* a, b, c, α, β and γ . Here a, b, c are the lengths of the basis vectors $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ and α, β and γ are the angles between \mathbf{a}_2 and $\mathbf{a}_3, \mathbf{a}_3$ and $\mathbf{a}_1, \mathbf{a}_1$ and \mathbf{a}_2 , respectively. The *metric matrix* \mathbf{M} (called \mathbf{G} in *IT A*, Chapter 9.1) is the (3×3) matrix which consists of the scalar products of the basis vectors:

$$\mathbf{M} = \begin{pmatrix} a^2 & ab \cos \gamma & ac \cos \beta \\ ba \cos \gamma & b^2 & bc \cos \alpha \\ ca \cos \beta & cb \cos \alpha & c^2 \end{pmatrix}.$$

If \mathbf{W} is the matrix part of an isometry, referred to the basis $(\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3)$, then \mathbf{W} must fulfil the condition $\mathbf{W}^T \mathbf{M} \mathbf{W} = \mathbf{M}$, where \mathbf{W}^T is the transpose of \mathbf{W} .

- (2) For the *determinant* of \mathbf{W} , $\det(\mathbf{W}) = \pm 1$ must hold; $\det(\mathbf{W}) = +1$ for the identity, translations, rotations and screw rotations; $\det(\mathbf{W}) = -1$ for inversions, reflections, glide reflections and rotoinversions.
- (3) For the *trace*, $\text{tr}(\mathbf{W}) = W_{11} + W_{22} + W_{33} = \pm(1 + 2 \cos \varphi)$ holds, where φ is the rotation angle; the $+$ sign applies if $\det(\mathbf{W}) = +1$ and the $-$ sign if $\det(\mathbf{W}) = -1$.

Algorithms for the determination of the kind of isometry from a given matrix–column pair and for the determination of the matrix–column pair for a given isometry can be found in *IT A*, Part 11 or in Hahn & Wondratschek (1994).

1.2.2.6. Vectors and vector coefficients

In crystallography, vectors and their coefficients as well as points and their coordinates are used for the description of crystal structures. Vectors represent translation shifts, distance and Patterson vectors, reciprocal-lattice vectors *etc.* With respect to a given basis a vector has three coefficients. In contrast to the coordinates of a point, these coefficients do not change if the origin of the coordinate system is shifted. In the usual description by columns, the vector coefficients cannot be distinguished from the point coordinates, but in the augmented-column description the difference becomes visible: the vector from the point P to the point Q has the coefficients $v_1 = q_1 - p_1, v_2 = q_2 - p_2, v_3 = q_3 - p_3, 1 - 1$. Thus, the column of the coefficients of a vector is not augmented by ‘1’ but by ‘0’. Therefore, when the point P is mapped onto the point \tilde{P} by $\tilde{\mathbf{x}} = \mathbf{W}\mathbf{x} + \mathbf{w}$ according to equation (1.2.2.3), then the vector $\mathbf{v} = \overrightarrow{PQ}$ is mapped onto the vector $\tilde{\mathbf{v}} = \overrightarrow{\tilde{P}\tilde{Q}}$ by transforming its coefficients by $\tilde{\mathbf{v}} = \mathbf{W}\mathbf{v}$, because the coefficients w_j are multiplied by the number ‘0’ augmenting the column $\mathbf{v} = (v_j)$. Indeed, the

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distance vector $\mathbf{v} = \overrightarrow{PQ}$ is not changed when the whole space is mapped onto itself by a translation.

Remarks:

- (1) The difference in transformation behaviour between the point coordinates \mathbf{x} and the vector coefficients \mathbf{v} is not visible in the equations where the symbols \mathbf{x} and \mathbf{v} are used, but is obvious only if the columns are written in full, *viz*

$$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \mathbf{1} \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} v_1 \\ v_2 \\ v_3 \\ 0 \end{pmatrix}.$$

- (2) The transformation behaviour of the vector coefficients is also apparent if the vector is understood to be a translation vector and the transformation behaviour of the translation is considered as in the last paragraph of the next section.
- (3) The transformation $\tilde{\mathbf{v}} = \mathbf{W}\mathbf{v}$ is called an *orthogonal mapping* if \mathbf{W} is the matrix part of an isometry.

1.2.2.7. Origin shift and change of the basis

It is in general advantageous to refer crystallographic objects and their symmetries to the most appropriate coordinate system. The best coordinate system may be different for different steps of the calculations and for different objects which have to be considered simultaneously. Therefore, a change of the origin and/or the basis are frequently necessary when treating crystallographic problems. Here the formulae for the influence of an origin shift and a change of basis on the matrix–column pairs of mappings and on the vector coefficients are only stated; the equations are derived in detail in *IT A* Chapters 5.2 and 5.3, and in Hahn & Wondratschek (1994).

Let a coordinate system be given with a basis $(\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3)^T$ and an origin O .¹ Referred to this coordinate system, the column of coordinates of a point P is \mathbf{x} ; the matrix and column parts describing a symmetry operation are \mathbf{W} and \mathbf{w} according to equations (1.2.2.1) to (1.2.2.3), and the column of vector coefficients is \mathbf{v} , see Section 1.2.2.6. A new coordinate system may be introduced with the basis $(\mathbf{a}'_1, \mathbf{a}'_2, \mathbf{a}'_3)^T$ and the origin O' . Referred to the new coordinate system, the column of coordinates of the point P is \mathbf{x}' , the symmetry operation is described by \mathbf{W}' and \mathbf{w}' and the column of vector coefficients is \mathbf{v}' .

Let $\mathbf{p} = \overrightarrow{OO'}$ be the column of coefficients for the vector from the old origin O to the new origin O' and let

$$\mathbf{P} = \begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix} \quad (1.2.2.9)$$

be the matrix of a basis change, *i.e.* the matrix that relates the new basis $(\mathbf{a}'_1, \mathbf{a}'_2, \mathbf{a}'_3)^T$ to the old basis $(\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3)^T$ according to

$$(\mathbf{a}'_1, \mathbf{a}'_2, \mathbf{a}'_3)^T = (\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3)^T \mathbf{P} = (\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3)^T \begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix}. \quad (1.2.2.10)$$

¹ In this volume, point coordinates and vector coefficients are thought of as columns in matrix multiplication. Therefore, columns are considered to be ‘standard’. These ‘columns’ are not marked, even if they are written in a row. To comply with the rules of matrix multiplication, rows are also introduced. These rows of symbols (*e.g.* vector coefficients of reciprocal space, *i.e.* Miller indices, or a set of basis vectors of direct space) are ‘transposed relative to columns’ and are, therefore, marked $(h, k, l)^T$ or $(\mathbf{a}, \mathbf{b}, \mathbf{c})^T$, even if they are written in a row.

Then the following equations hold:

$$\mathbf{x}' = \mathbf{P}^{-1}\mathbf{x} - \mathbf{P}^{-1}\mathbf{p} \quad \text{or} \quad \mathbf{x} = \mathbf{P}\mathbf{x}' + \mathbf{p}; \quad (1.2.2.11)$$

$$\mathbf{W}' = \mathbf{P}^{-1}\mathbf{W}\mathbf{P} \quad \text{or} \quad \mathbf{W} = \mathbf{P}\mathbf{W}'\mathbf{P}^{-1}; \quad (1.2.2.12)$$

$$\mathbf{w}' = \mathbf{P}^{-1}(\mathbf{w} + (\mathbf{W} - \mathbf{I})\mathbf{p}) \quad \text{or} \quad \mathbf{w} = \mathbf{P}\mathbf{w}' - (\mathbf{W} - \mathbf{I})\mathbf{p}. \quad (1.2.2.13)$$

For the columns of vector coefficients \mathbf{v} and \mathbf{v}' , the following holds:

$$\mathbf{v}' = \mathbf{P}^{-1}\mathbf{v} \quad \text{or} \quad \mathbf{v} = \mathbf{P}\mathbf{v}', \quad (1.2.2.14)$$

i.e. an origin shift does not change the vector coefficients.

These equations read in the augmented-matrix formalism

$$\mathbf{x}' = \mathbf{P}^{-1}\mathbf{x}; \quad \mathbf{W}' = \mathbf{P}^{-1}\mathbf{W}\mathbf{P}; \quad \mathbf{v}' = \mathbf{P}^{-1}\mathbf{v}. \quad (1.2.2.15)$$

For the difference in the transformation behaviour of point coordinates and vector coefficients, see the remarks at the end of Section 1.2.2.6. A vector \mathbf{v} can be regarded as a translation vector; its translation is then described by (\mathbf{I}, \mathbf{v}) , *i.e.* $\mathbf{W} = \mathbf{I}$, $\mathbf{w} = \mathbf{v}$. It can be shown using equation (1.2.2.13) that the translation and thus the translation vector are not changed under an origin shift, (\mathbf{I}, \mathbf{p}) , because $(\mathbf{I}, \mathbf{v})' = (\mathbf{I}, \mathbf{v})$ holds. Moreover, under a general coordinate transformation the origin shift is not effective: in equation (1.2.2.13) only $\mathbf{v}' = \mathbf{P}^{-1}\mathbf{v}$ remains because of the equality $\mathbf{W} = \mathbf{I}$.

1.2.3. Groups

Group theory is the proper tool for studying symmetry in science. The symmetry group of an object is the set of all isometries (rigid motions) which map that object onto itself. If the object is a crystal, the isometries which map it onto itself (and also leave it invariant as a whole) are the *crystallographic symmetry operations*.

There is a huge amount of literature on group theory and its applications. The book *Introduction to Group Theory* by Ledermann (1976) is recommended. The book *Symmetry of Crystals. Introduction to International Tables for Crystallography, Vol. A* by Hahn & Wondratschek (1994) describes a way in which the data of *IT A* can be interpreted by means of matrix algebra and elementary group theory. It may also help the reader of this volume.

1.2.3.1. Some properties of symmetry groups

The geometric symmetry of any object is described by a group \mathcal{G} . The symmetry operations $g_j \in \mathcal{G}$ are the group elements, and the set $\{g_j \in \mathcal{G}\}$ of all symmetry operations fulfils the group postulates. [A ‘symmetry element’ in crystallography is not a group element of a symmetry group but is a combination of a geometric object with that set of symmetry operations which leave the geometric object invariant, *e.g.* an axis with its threefold rotations or a plane with its glide reflections *etc.*, *cf.* Flack *et al.* (2000).] Groups will be designated by upper-case calligraphic script letters \mathcal{G} , \mathcal{H} *etc.* Group elements are represented by lower-case slanting *sans serif* letters g, h *etc.*

The result g_r of the composition of two elements $g_j, g_k \in \mathcal{G}$ will be called the *product* of g_j and g_k and will be written $g_r = g_k g_j$. The first operation is the right factor because the point coordinates or vector coefficients are written as columns on which the matrices of the symmetry operations are applied from the left side.

The *law of composition* in the group is the successive application of the symmetry operations.

The *group postulates* are shown to hold for symmetry groups:

- (1) The *closure*, *i.e.* the property that the composition of any two symmetry operations results in a symmetry operation again, is always fulfilled for geometric symmetries: if $g_j \in \mathcal{G}$ and $g_k \in \mathcal{G}$, then $g_j g_k = g_r \in \mathcal{G}$ also holds.

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- (2) The *associative law* is always fulfilled for the composition of geometric mappings. If $g_j, g_k, g_m \in \mathcal{G}$, then $(g_j g_k) g_m = g_j (g_k g_m) = g_q$ for any triplet j, k, m . Therefore, the parentheses are not necessary, one can write $g_j g_k g_m = g_q$. In general, however, the sequence of the symmetry operations must not be changed. Thus, in general $g_j g_k g_m \neq g_j g_m g_k$.
- (3) The *unit element* or *neutral element* $e \in \mathcal{G}$ is the identity operation which maps each point onto itself, *i.e.* leaves each point invariant.
- (4) The isometry which reverses a given symmetry operation $g \in \mathcal{G}$ is also a symmetry operation of \mathcal{G} and is called the *inverse* symmetry operation g^{-1} of g . It has the property $g g^{-1} = g^{-1} g = e$.

The number of elements of a group \mathcal{G} is called its *order* $|\mathcal{G}|$. The order of a group may be finite, *e.g.* 24 for the symmetry operations of a regular tetrahedron, or infinite, *e.g.* for any space group because of its infinite set of translations. If the relation $g_k g_j = g_j g_k$ is fulfilled for all pairs of elements of a group \mathcal{G} , then \mathcal{G} is called a *commutative* or an *Abelian* group.

For groups of higher order, it is usually inappropriate and for groups of infinite order it is impossible to list all elements of a group. The following definition nearly always reduces the set of group elements to be listed explicitly to a small set.

Definition 1.2.3.1.1. A set $\mathcal{S} = \{g_p, g_q, \dots\} \in \mathcal{G}$ such that every element of \mathcal{G} can be obtained by composition of the elements of \mathcal{S} and their inverses is called a *set of generators* of \mathcal{G} . The elements $g_i \in \mathcal{S}$ are called *generators* of \mathcal{G} . \square

A group is *cyclic* if it consists of the unit element e and all powers of one element g :

$$\mathcal{C}(g) = \{\dots g^{-3}, g^{-2}, g^{-1}, e, g^1, g^2, g^3, \dots\}.$$

If there is an integer number $n > 0$ with $g^n = e$ and n is the smallest number with this property, then the group $\mathcal{C}(g)$ has the *finite order* n . Let g^{-k} with $0 < k < n$ be the inverse element of g^k where n is the order of g . Because $g^{-k} = g^n g^{-k} = g^{n-k} = g^m$ with $n = m + k$, the elements of a cyclic group of finite order can all be written as positive powers of the generator g . Otherwise, if such an integer n does not exist, the group $\mathcal{C}(g)$ is of *infinite order* and the positive powers g^k are different from the negative ones g^{-m} .

In the same way, from any element $g_j \in \mathcal{G}$ its cyclic group $\mathcal{C}(g_j)$ can be generated even if \mathcal{G} is not cyclic itself. The order of this group $\mathcal{C}(g_j)$ is called the *order of the element* g_j .

1.2.3.2. Group isomorphism and homomorphism

A finite group \mathcal{G} of small order may be conveniently visualized by its *multiplication table*, *group table* or *Cayley table*. An example is shown in Table 1.2.3.1.

The multiplication tables can be used to define one of the most important relations between two groups, the isomorphism of groups. This can be done by comparing the multiplication tables of the two groups.

Definition 1.2.3.2.1. Two groups are *isomorphic* if one can arrange the rows and columns of their multiplication tables such that these tables are equal, apart from the names or symbols of the group elements. \square

Multiplication tables are useful only for groups of small order. To define ‘isomorphism’ for arbitrary groups, one can formu-

Table 1.2.3.1. *Multiplication table of a group*

The group elements $g \in \mathcal{G}$ are listed at the top of the table and in the same sequence on the left-hand side; the unit element ‘ e ’ is listed first. The table is thus a square array. The product $g_k g_j$ of any pair of elements is listed at the intersection of the k th row and the j th column.

It can be shown that each group element is listed exactly once in each row and once in each column of the table. In the row of an element $g \in \mathcal{G}$, the unit element e appears in the column of g^{-1} . If $(g)^2 = e$, *i.e.* $g = g^{-1}$, e appears on the main diagonal. The multiplication table of an Abelian group is symmetric about the main diagonal.

\mathcal{G}	e	a	b	c	\dots
e	e	a	b	c	\dots
a	a	a^2	ab	ac	\dots
b	b	ba	b^2	bc	\dots
c	c	ca	cb	c^2	\dots
\vdots	\vdots	\vdots	\vdots	\vdots	\ddots

late the relations expressed by the multiplication tables in a more abstract way.

The ‘same multiplication table’ for the groups \mathcal{G} and \mathcal{G}' means that there is a reversible mapping $g_q \longleftrightarrow g'_q$ of the elements $g_q \in \mathcal{G}$ and $g'_q \in \mathcal{G}'$ such that $(g_j g_k)' = g'_j g'_k$ holds for any pair of indices j and k . In words:

Definition 1.2.3.2.2. Two groups \mathcal{G} and \mathcal{G}' are *isomorphic* if there is a reversible mapping of \mathcal{G} onto \mathcal{G}' such that for any pair of elements of \mathcal{G} the image of the product is equal to the product of the images. \square

Isomorphic groups have the same order. By isomorphism the set of all groups is classified into *isomorphism types* or *isomorphism classes* of groups. Such a class is often called an *abstract group*.

The isomorphism between the space groups and the corresponding matrix groups makes an analytical treatment of crystallographic symmetry possible. Moreover, the isomorphism of different space groups allows one to classify the infinite number of space groups into a finite number of *isomorphism types of space groups*, which is one of the bases of crystallography, see Section 1.2.5.

Isomorphism provides a very strong relation between groups: the groups are identical in their group-theoretical properties. One can weaken this relation by omitting the condition of reversibility of the mapping. One then admits that more than one element of the group \mathcal{G} is mapped onto the same element of \mathcal{G}' . This concept leads to the definition of homomorphism.

Definition 1.2.3.2.3. A mapping of a group \mathcal{G} onto a group \mathcal{G}' is called *homomorphic*, and \mathcal{G}' is called a *homomorphic image* of the group \mathcal{G} , if for any pair of elements of \mathcal{G} the image of the product is equal to the product of the images and if any element of \mathcal{G}' is the image of at least one element of \mathcal{G} . The relation of \mathcal{G} and \mathcal{G}' is called a *homomorphism*. More formally: For the mapping \mathcal{G} onto \mathcal{G}' , $(g_j g_k)' = g'_j g'_k$ holds. \square

The formulation ‘mapping onto’ implies that each element $g' \in \mathcal{G}'$ occurs among the images of the elements $g \in \mathcal{G}$ at least once.²

The very important concept of homomorphism is discussed further in Lemma 1.2.4.4.3. The crystallographic point groups are homomorphic images of the space groups, see Section 1.2.5.4.

² In mathematics, the term ‘homomorphism’ includes mappings of a group \mathcal{G} into a group \mathcal{G}' , *i.e.* mappings in which not every $g' \in \mathcal{G}'$ is the image of some element of $g \in \mathcal{G}$. The term ‘homomorphism onto’ defined above is also known as an *epimorphism*, *e.g.* in Ledermann (1976). In the older literature the term ‘multiple isomorphism’ can also be found.

1.2.4. Subgroups

1.2.4.1. Definition

There may be sets of elements $g_k \in \mathcal{G}$ that do not constitute the full group \mathcal{G} but nevertheless fulfil the group postulates for themselves.

Definition 1.2.4.1.1. A subset \mathcal{H} of elements of a group \mathcal{G} is called a *subgroup* \mathcal{H} of \mathcal{G} if it fulfils the group postulates with respect to the law of composition of \mathcal{G} . \square

Remarks:

- (1) The group \mathcal{G} is considered to be one of its own subgroups. If subgroups \mathcal{H}_j are discussed where \mathcal{G} is included among the subgroups, we write $\mathcal{H}_j \leq \mathcal{G}$ or $\mathcal{G} \geq \mathcal{H}_j$. If \mathcal{G} is excluded from the set $\{\mathcal{H}_j\}$ of its subgroups, we write $\mathcal{H}_j < \mathcal{G}$ or $\mathcal{G} > \mathcal{H}_j$. A subgroup $\mathcal{H}_j < \mathcal{G}$ is called a *proper subgroup* of \mathcal{G} .
- (2) In a relation $\mathcal{G} \geq \mathcal{H}$ or $\mathcal{G} > \mathcal{H}$, \mathcal{G} is called a *supergroup* of \mathcal{H} . The symbols \leq , \geq , $<$ and $>$ are used for supergroups in the same way as they are used for subgroups, cf. Section 2.1.6.
- (3) A subgroup of a finite group is finite. A subgroup of an infinite group may be finite or infinite.
- (4) A subset \mathcal{K} of elements $g_k \in \mathcal{G}$ which does not necessarily form a group is designated by the symbol $\mathcal{K} \subset \mathcal{G}$.

Definition 1.2.4.1.2. A subgroup $\mathcal{H} < \mathcal{G}$ is a *maximal subgroup* if no group \mathcal{Z} exists for which $\mathcal{H} < \mathcal{Z} < \mathcal{G}$ holds. If \mathcal{H} is a maximal subgroup of \mathcal{G} , then \mathcal{G} is a *minimal supergroup* of \mathcal{H} . \square

This definition is very important for the tables of this volume, as only maximal subgroups of space groups are listed. If all maximal subgroups are known for any given space group, then any general subgroup $\mathcal{H} < \mathcal{G}$ can be obtained by a (finite) chain of maximal subgroups between \mathcal{G} and \mathcal{H} , see Section 1.2.6.2. Moreover, the relations between a space group and its maximal subgroups are particularly transparent, cf. Lemma 1.2.8.1.3.

1.2.4.2. Coset decomposition and normal subgroups

Let $\mathcal{H} < \mathcal{G}$ be a subgroup of \mathcal{G} of order $|\mathcal{H}|$. Because \mathcal{H} is a proper subgroup of \mathcal{G} there must be elements $g_q \in \mathcal{G}$ that are not elements of \mathcal{H} . Let $g_2 \in \mathcal{G}$ be one of them. Then the set of elements $g_2\mathcal{H} = \{g_2 h_j | h_j \in \mathcal{H}\}$ ³ is a subset of elements of \mathcal{G} with the property that all its elements are different and that the sets \mathcal{H} and $g_2\mathcal{H}$ have no element in common. Thus, the set $g_2\mathcal{H}$ also contains $|\mathcal{H}|$ elements of \mathcal{G} . If there is another element $g_3 \in \mathcal{G}$ which belongs neither to \mathcal{H} nor to $g_2\mathcal{H}$, one can form another set $g_3\mathcal{H} = \{g_3 h_j | h_j \in \mathcal{H}\}$. All elements of $g_3\mathcal{H}$ are different and none occurs already in \mathcal{H} or in $g_2\mathcal{H}$. This procedure can be continued until each element $g_r \in \mathcal{G}$ belongs to one of these sets. In this way the group \mathcal{G} can be partitioned, such that each element $g \in \mathcal{G}$ belongs to exactly one of these sets.

Definition 1.2.4.2.1. The partition just described is called a *decomposition* $(\mathcal{G} : \mathcal{H})$ into *left cosets* of the group \mathcal{G} relative to the group \mathcal{H} . The sets $g_p\mathcal{H}$, $p = 1, \dots, i$ are called *left cosets*, because the elements $h_j \in \mathcal{H}$ are multiplied with the new elements from the left-hand side. The procedure is called a *decomposition into right cosets* $\mathcal{H}g_s$ if the elements $h_j \in \mathcal{H}$ are multiplied with the new elements g_s from the right-hand side. The elements g_p or

g_s are called the *coset representatives*. The number of cosets is called the *index* $i = |\mathcal{G} : \mathcal{H}|$ of \mathcal{H} in \mathcal{G} . \square

Remarks:

- (1) The group $\mathcal{H} = g_1\mathcal{H}$ with $g_1 = e$ is the first coset for both kinds of decomposition. It is the only coset which forms a group by itself.
- (2) All cosets have the same *length*, i.e. the same number of elements, which is equal to $|\mathcal{H}|$, the order of \mathcal{H} .
- (3) The index i is the same for both right and left decompositions. In IT A and in this volume, the index is frequently designated by the symbol $[i]$.
- (4) A coset does not depend on its representative element; starting from any of its elements will result in the same coset. The right cosets may be different from the left ones and the representatives of the right and left cosets may also differ.
- (5) If the order $|\mathcal{G}|$ of \mathcal{G} is infinite, then either the order $|\mathcal{H}|$ of \mathcal{H} or the index $i = |\mathcal{G} : \mathcal{H}|$ of \mathcal{H} in \mathcal{G} or both are infinite.
- (6) The coset decomposition of a space group \mathcal{G} relative to its translation subgroup $\mathcal{T}(\mathcal{G})$ is fundamental in crystallography, cf. Section 1.2.5.4.

From its definition and from the properties of the coset decomposition mentioned above, one immediately obtains the fundamental theorem of Lagrange (for another formulation, see Chapter 1.5):

Lemma 1.2.4.2.2. *Lagrange's theorem:* Let \mathcal{G} be a group of finite order $|\mathcal{G}|$ and $\mathcal{H} < \mathcal{G}$ a subgroup of \mathcal{G} of order $|\mathcal{H}|$. Then $|\mathcal{H}|$ is a divisor of $|\mathcal{G}|$ and the equation $|\mathcal{H}| \times i = |\mathcal{G}|$ holds where $i = |\mathcal{G} : \mathcal{H}|$ is the index of \mathcal{H} in \mathcal{G} . \square

A special situation exists when the left and right coset decompositions of \mathcal{G} relative to \mathcal{H} result in the partition of \mathcal{G} into the same cosets:

$$g_p\mathcal{H} = \mathcal{H}g_p \text{ for all } 1 \leq p \leq i. \quad (1.2.4.1)$$

Subgroups \mathcal{H} that fulfil equation (1.2.4.1) are called ‘normal subgroups’ according to the following definition:

Definition 1.2.4.2.3. A subgroup $\mathcal{H} < \mathcal{G}$ is called a *normal subgroup* or *invariant subgroup* of \mathcal{G} , $\mathcal{H} \triangleleft \mathcal{G}$, if equation (1.2.4.1) is fulfilled. \square

The relation $\mathcal{H} \triangleleft \mathcal{G}$ always holds for $|\mathcal{G} : \mathcal{H}| = 2$, i.e. subgroups of index 2 are always normal subgroups. The subgroup \mathcal{H} contains half of the elements of \mathcal{G} , whereas the other half of the elements forms ‘the other’ coset. This coset must then be the right as well as the left coset.

1.2.4.3. Conjugate elements and conjugate subgroups

In a coset decomposition, the set of all elements of the group \mathcal{G} is partitioned into cosets which form classes in the mathematical sense of the word, i.e. each element of \mathcal{G} belongs to exactly one coset.

Another equally important partition of the group \mathcal{G} into classes of elements arises from the following definition:

Definition 1.2.4.3.1. Two elements $g_j, g_k \in \mathcal{G}$ are called *conjugate* if there is an element $g_q \in \mathcal{G}$ such that $g_q^{-1}g_jg_q = g_k$. \square

Remarks:

- (1) Definition 1.2.4.3.1 partitions the elements of \mathcal{G} into classes of conjugate elements which are called *conjugacy classes of elements*.
- (2) The unit element always forms a conjugacy class by itself.

³ The formulation $g_2\mathcal{H} = \{g_2 h_j | h_j \in \mathcal{H}\}$ means: ‘ $g_2\mathcal{H}$ is the set of the products $g_2 h_j$ of g_2 with all elements $h_j \in \mathcal{H}$.’

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- (3) Each element of an Abelian group forms a conjugacy class by itself.
- (4) Elements of the same conjugacy class have the same order.
- (5) Different conjugacy classes may contain different numbers of elements, *i.e.* have different ‘lengths’.

Not only the individual elements of a group \mathcal{G} but also the subgroups of \mathcal{G} can be classified in conjugacy classes.

Definition 1.2.4.3.2. Two subgroups $\mathcal{H}_j, \mathcal{H}_k < \mathcal{G}$ are called *conjugate* if there is an element $g_q \in \mathcal{G}$ such that $g_q^{-1} \mathcal{H}_j g_q = \mathcal{H}_k$ holds. This relation is often written $\mathcal{H}_j^{g_q} = \mathcal{H}_k$. \square

Remarks:

- (1) The ‘trivial subgroup’ \mathcal{I} (consisting only of the unit element of \mathcal{G}) and the group \mathcal{G} itself each form a conjugacy class by themselves.
- (2) Each subgroup of an Abelian group forms a conjugacy class by itself.
- (3) Subgroups in the same conjugacy class are isomorphic and thus have the same order.
- (4) Different conjugacy classes of subgroups may contain different numbers of subgroups, *i.e.* have different lengths.

Equation (1.2.4.1) can be written

$$\mathcal{H} = g_p^{-1} \mathcal{H} g_p \text{ or } \mathcal{H} = \mathcal{H}^{g_p} \text{ for all } p; 1 \leq p \leq i. \quad (1.2.4.2)$$

Using conjugation, Definition 1.2.4.2.3 can be formulated as

Definition 1.2.4.3.3. A subgroup \mathcal{H} of a group \mathcal{G} is a normal subgroup $\mathcal{H} \triangleleft \mathcal{G}$ if it is identical with all of its conjugates, *i.e.* if its conjugacy class consists of the one subgroup \mathcal{H} only. \square

1.2.4.4. Factor groups and homomorphism

For the following definition, the ‘product of sets of group elements’ will be used:

Definition 1.2.4.4.1. Let \mathcal{G} be a group and $\mathcal{K}_j = \{g_{j_1}, \dots, g_{j_n}\}$, $\mathcal{K}_k = \{g_{k_1}, \dots, g_{k_m}\}$ be two arbitrary sets of its elements which are not necessarily groups themselves. Then the product $\mathcal{K}_j \mathcal{K}_k$ of \mathcal{K}_j and \mathcal{K}_k is the set of all products $\mathcal{K}_j \mathcal{K}_k = \{g_{j_p} g_{k_q} \mid g_{j_p} \in \mathcal{K}_j, g_{k_q} \in \mathcal{K}_k\}$.⁴ \square

The coset decomposition of a group \mathcal{G} relative to a normal subgroup $\mathcal{H} \triangleleft \mathcal{G}$ has a property which makes it particularly useful for displaying the structure of a group.

Consider the coset decomposition with the cosets \mathcal{S}_j and \mathcal{S}_k of a group \mathcal{G} relative to its subgroup $\mathcal{H} < \mathcal{G}$. In general the product $\mathcal{S}_j \mathcal{S}_k$ of two cosets, *cf.* Definition 1.2.4.4.1, will not be a coset again. However, if and only if $\mathcal{H} \triangleleft \mathcal{G}$ is a normal subgroup of \mathcal{G} , the product of two cosets is always another coset. This means that for the set of all cosets of a normal subgroup $\mathcal{H} \triangleleft \mathcal{G}$ there exists a law of composition for which the closure is fulfilled. One can show that the other group postulates are also fulfilled for the cosets and their multiplication if $\mathcal{H} \triangleleft \mathcal{G}$ holds: there is a neutral element (which is \mathcal{H}), for each coset $g\mathcal{H} = \mathcal{H}g$ the coset $g^{-1}\mathcal{H} = \mathcal{H}g^{-1}$ forms the inverse element and for the coset multiplication the associative law holds.

Definition 1.2.4.4.2. Let $\mathcal{H} \triangleleft \mathcal{G}$. The cosets of the decomposition of the group \mathcal{G} relative to the normal subgroup $\mathcal{H} \triangleleft \mathcal{G}$ form a group with respect to the composition law of coset multiplication. This

⁴ The right-hand side of this equation is the set of all products $g_r = g_{j_p} g_{k_q}$, where g_{j_p} runs through all elements of \mathcal{K}_j and g_{k_q} through all elements of \mathcal{K}_k . Each element g_r is taken only once in the set.

group is called the *factor group* \mathcal{G}/\mathcal{H} . Its order is $|\mathcal{G} : \mathcal{H}|$, *i.e.* the index of \mathcal{H} in \mathcal{G} . \square

A factor group $\mathcal{F} = \mathcal{G}/\mathcal{H}$ is not necessarily isomorphic to a subgroup $\mathcal{H}_j < \mathcal{G}$.

Factor groups are indispensable for an understanding of the homomorphism of one group onto the other. The relations between a group \mathcal{G} and its homomorphic image are very strong and are expressed by the following lemma:

Lemma 1.2.4.4.3. Let \mathcal{G}' be a homomorphic image of the group \mathcal{G} . Then the set of all elements of \mathcal{G} that are mapped onto the unit element $e' \in \mathcal{G}'$ forms a normal subgroup \mathcal{X} of \mathcal{G} . The group \mathcal{G}' is isomorphic to the factor group \mathcal{G}/\mathcal{X} and the cosets of \mathcal{X} in \mathcal{G} are mapped onto the elements of \mathcal{G}' . The normal subgroup \mathcal{X} is called the *kernel* of the mapping; it forms the unit element of the factor group \mathcal{G}/\mathcal{X} . A homomorphic image of \mathcal{G} exists for any normal subgroup of \mathcal{G} . \square

The most important homomorphism in crystallography is the relation between a space group \mathcal{G} and its homomorphic image, the point group \mathcal{P} , where the kernel is the subgroup $\mathcal{T}(\mathcal{G})$ of all translations of \mathcal{G} , *cf.* Section 1.2.5.4.

1.2.4.5. Normalizers

The concept of the normalizer $\mathcal{N}_{\mathcal{G}}(\mathcal{H})$ of a group $\mathcal{H} < \mathcal{G}$ in a group \mathcal{G} is very useful for the considerations of the following sections. The size of the conjugacy class of \mathcal{H} in \mathcal{G} is determined by this normalizer.

Let $\mathcal{H} < \mathcal{G}$ and $h_j \in \mathcal{H}$. Then $h_j^{-1} \mathcal{H} h_j = \mathcal{H}$ holds because \mathcal{H} is a group. If $\mathcal{H} \triangleleft \mathcal{G}$, then $g_k^{-1} \mathcal{H} g_k = \mathcal{H}$ for any $g_k \in \mathcal{G}$. If \mathcal{H} is not a normal subgroup of \mathcal{G} , there may nevertheless be elements $g_p \in \mathcal{G}$, $g_p \notin \mathcal{H}$ for which $g_p^{-1} \mathcal{H} g_p = \mathcal{H}$ holds. We consider the set of all elements $g_p \in \mathcal{G}$ that have this property.

Definition 1.2.4.5.1. The set of all elements $g_p \in \mathcal{G}$ that map the subgroup $\mathcal{H} < \mathcal{G}$ onto itself by conjugation, $\mathcal{H} = g_p^{-1} \mathcal{H} g_p = \mathcal{H}^{g_p}$, forms a group $\mathcal{N}_{\mathcal{G}}(\mathcal{H})$, called the *normalizer of \mathcal{H} in \mathcal{G}* , where $\mathcal{H} \triangleleft \mathcal{N}_{\mathcal{G}}(\mathcal{H}) \leq \mathcal{G}$. \square

Remarks:

- (1) The group $\mathcal{H} < \mathcal{G}$ is a normal subgroup of \mathcal{G} , $\mathcal{H} \triangleleft \mathcal{G}$, if and only if $\mathcal{N}_{\mathcal{G}}(\mathcal{H}) = \mathcal{G}$.
- (2) Let $\mathcal{N}_{\mathcal{G}}(\mathcal{H}) = \{g_p\}$. One can decompose \mathcal{G} into right cosets relative to $\mathcal{N}_{\mathcal{G}}(\mathcal{H})$. All elements $g_p g_r$ of a right coset $\mathcal{N}_{\mathcal{G}}(\mathcal{H}) g_r$ of this decomposition ($\mathcal{G} : \mathcal{N}_{\mathcal{G}}(\mathcal{H})$) transform \mathcal{H} into the same subgroup $g_r^{-1} g_p^{-1} \mathcal{H} g_p g_r = g_r^{-1} \mathcal{H} g_r < \mathcal{G}$, which is thus conjugate to \mathcal{H} in \mathcal{G} by g_r .
- (3) The elements of different cosets of ($\mathcal{G} : \mathcal{N}_{\mathcal{G}}(\mathcal{H})$) transform \mathcal{H} into different conjugates of \mathcal{H} . The number of cosets of $\mathcal{N}_{\mathcal{G}}(\mathcal{H})$ is equal to the index $i_N = |\mathcal{G} : \mathcal{N}_{\mathcal{G}}(\mathcal{H})|$ of $\mathcal{N}_{\mathcal{G}}(\mathcal{H})$ in \mathcal{G} . Therefore, the number $N_{\mathcal{H}}$ of conjugates in the conjugacy class of \mathcal{H} is equal to the index i_N and is thus determined by the order of $\mathcal{N}_{\mathcal{G}}(\mathcal{H})$. From $\mathcal{N}_{\mathcal{G}}(\mathcal{H}) \geq \mathcal{H}$, $i_N = |\mathcal{G} : \mathcal{N}_{\mathcal{G}}(\mathcal{H})| \leq |\mathcal{G} : \mathcal{H}| = i$ follows. This means that the number of conjugates of a subgroup $\mathcal{H} < \mathcal{G}$ cannot exceed the index $i = |\mathcal{G} : \mathcal{H}|$.
- (4) If $\mathcal{H} < \mathcal{G}$ is a maximal subgroup of \mathcal{G} , then either $\mathcal{N}_{\mathcal{G}}(\mathcal{H}) = \mathcal{G}$ and $\mathcal{H} \triangleleft \mathcal{G}$ is a normal subgroup of \mathcal{G} or $\mathcal{N}_{\mathcal{G}}(\mathcal{H}) = \mathcal{H}$ and the number of conjugates is equal to the index $i = |\mathcal{G} : \mathcal{H}|$.
- (5) For the normalizers of the space groups, see the corresponding part of Section 1.2.6.3.

1.2.5. Space groups

1.2.5.1. Space groups and their description

The set of all symmetry operations of a three-dimensional crystal pattern, *i.e.* its symmetry group, is the *space group* of this crystal pattern. In a plane, the symmetry group of a two-dimensional crystal pattern is its *plane group*. In the following, the term ‘space group’ alone will be used and the plane groups are included because they are the space groups of two-dimensional space.

A crystal pattern is a periodic array. This means that there are translations among its symmetry operations. The translations of crystals are small (a few angströms to a few hundred angströms) but cannot be arbitrarily short because of the finite size of the particles in crystal structures. One thus defines for any finite integer n :

Definition 1.2.5.1.1. A group \mathcal{G} of isometries in n -dimensional space is called an n -dimensional space group if

- (1) \mathcal{G} contains n linearly independent translations.
- (2) There is a minimum length $\delta > 0$ such that the length r of any translation vector is at least $r = \delta$. \square

Condition (2) is justified because crystal structures contain atoms of finite size, and it is necessary to avoid infinitely small translations as elements of space groups. Several fundamental properties would not hold without this condition, such as the existence of a lattice of translation vectors and the restriction to only a few rotation angles.

In this volume, only the dimensions $n = 2$ and $n = 3$ will be dealt with. However, the space groups (more precisely, the space-group types, *cf.* Section 1.2.5.3) and other crystallographic items are also known for dimensions $n = 4$ and $n = 5$; the number of the affine space-group types is even known for $n = 6$: 28 927 922 (Plesken & Schulz, 2000).

One of the characteristics of a space group is its translation group. Any space group \mathcal{G} is an infinite group because the number of its translations is already infinite. The set of all translations of \mathcal{G} forms the infinite translation subgroup $\mathcal{T}(\mathcal{G}) \triangleleft \mathcal{G}$ with the composition law of performing one translation after the other, represented by the multiplication of matrix–column pairs. The group $\mathcal{T}(\mathcal{G})$ is a normal subgroup of \mathcal{G} of finite index. The vector lattice \mathbf{L} , *cf.* Section 1.2.2.2, forms a group with the composition law of vector addition. This group is isomorphic to the group $\mathcal{T}(\mathcal{G})$.

The matrix–column pairs of the symmetry operations of a space group \mathcal{G} are mostly referred to the *conventional coordinate system*. Its basis is chosen as a lattice basis and in such a way that the matrices for the linear parts of the symmetry operations of \mathcal{G} are particularly simple. The origin is chosen such that as many coset representatives as possible can be selected with their column coefficients to be zero, or such that the origin is situated on a centre of inversion. This means (for details and examples see Section 8.3.1 of *IT A*):

- (1) The basis is always chosen such that all matrix coefficients are 0 or ± 1 .
- (2) If possible, the basis is chosen such that all matrices have main diagonal form; then six of the nine coefficients are 0 and three are ± 1 .
- (3) If (2) is not possible, the basis is chosen such that the matrices are orthogonal. Again, six coefficients are 0 and three are ± 1 .
- (4) If (3) is not possible, the basis is hexagonal. At least five of the nine matrix coefficients are 0 and at most four are ± 1 .

- (5) The conventional basis chosen according to these rules is not always primitive, *cf.* the first example of Section 8.3.1 of *IT A*. If the conventional basis is primitive, then the lattice is also called *primitive*; if the conventional basis is not primitive, then the lattice referred to this (non-primitive) basis is called a *centred lattice*.
- (6) The matrix parts of a translation and of an inversion are

$$\mathbf{I} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \text{and} \quad \bar{\mathbf{I}} = \begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix},$$

i.e. the unit matrix and the negative unit matrix. They are independent of the basis.

- (7) The basis vectors of a crystallographic basis are lattice vectors. This makes the description of the lattice and of the symmetry operations of a crystal pattern independent of the actual metrics of the lattice, *e.g.* independent of temperature and pressure. It also means that the description of the symmetry may be the same for space groups of the same type, *cf.* Section 1.2.5.3.
- (8) The origin is chosen at a point of highest site symmetry which is left invariant by as many symmetry operations as possible. The column parts \mathbf{w}_k of these symmetry operations are $\mathbf{w}_k = \mathbf{o}$, *i.e.* the columns consist of zeroes only.

It is obviously impossible to list all elements of an infinite group individually. One could define the space group by a set of generators, because the number of necessary generators for any space group is finite: theoretically, up to six generators might be necessary but in practice up to ten generators are chosen for a space group. In *IT A* and in this volume, the set of the conventional generators is listed in the block ‘Generators selected’. The unit element is taken as the first generator; the generating translations follow and the generation is completed with the generators of the non-translation symmetry operations. The rules for the choice of the conventional generators are described in *IT A*, Section 8.3.5.

The description by generators is particularly important for this volume because many of the maximal subgroups in Chapters 2.2 and 2.3 are listed by their generators. These generators are chosen such that the generation of the general position can follow a *composition series*, *cf.* Ledermann (1976). This procedure allows the generation by a short program or even by hand. For details see *IT A*, Section 8.3.5; in Table 8.3.5.2 of *IT A* an example for the generation of a space group along these lines is displayed.

There are four ways to describe a space group in *IT A*:

- (i) A set of generators is the first way in which the space-group types \mathcal{G} , *cf.* Section 1.2.5.3, are described in *IT A*. This way is also used in the tables of this volume.
- (ii) By the matrices of the coset representatives of $(\mathcal{G} : \mathcal{T}(\mathcal{G}))$ in the general position. These matrices are not written in full but in a shorthand notation, *cf.* Section 8.1.5 or Chapter 11.1 of *IT A*. This kind of description is used for *translationengleiche* maximal subgroups in Chapters 2.2 and 2.3 of this volume, but in a slightly modified way, *cf.* Section 2.1.3.
- (iii) In a visual way by diagrams of the symmetry elements (not symmetry operations!) of \mathcal{G} within a unit cell and its surroundings.
- (iv) Also in a visual way by depicting the general-position points, again within a unit cell and its surroundings.

1. SPACE GROUPS AND THEIR SUBGROUPS

1.2.5.2. Classifications of space groups

There are an infinite number of space groups because there are an infinite number of known or conceivable crystals and crystal patterns. Indeed, because the lattice parameters depend on temperature and pressure, so do the lattice translations and the space group of a crystal. There is great interest in getting an overview of this vast number of space groups. To achieve this goal, one first characterizes the space groups by their group-theoretical properties and classifies them into space-group types where the space groups of each type have certain properties in common. To get a better overview, one then classifies the space-group types such that related types belong to the same ‘superclass’. This classification is done in two ways (*cf.* Sections 1.2.5.4 and 1.2.5.5):

- (1) first into *geometric crystal classes* by the point group of the space group, and then into *crystal systems*;
- (2) into the arithmetic crystal classes of the space groups and then into *Bravais flocks* and into *lattice systems* (not treated here, *cf.* *IT A*, Section 8.2.5);
- (3) all these classes: geometric and arithmetic crystal classes, crystal systems, Bravais flocks and lattice systems are classified into *crystal families*.

In reality, the tables in Chapters 2.2 and 2.3 and the graphs in Chapters 2.4 and 2.5 are tables and graphs for space-group types. The sequence of the space-group types in *IT A* and thus in this volume is determined by their crystal class, their crystal system and their crystal family. Therefore, these classifications are treated in the next sections. The point groups and the translation groups of the space groups can also be classified in a similar way. Only the classification of the point groups is treated in this chapter. For a more detailed treatment and for the classification of the lattices, the reader is referred to Chapter 1.5 of this volume, to Part 8 of *IT A* or to Brown *et al.* (1978).

1.2.5.3. Space groups and space-group types

We first consider the classification of the space groups into types. A more detailed treatment may be found in Section 8.2.1 of *IT A*. In practice, a common way is to look for the symmetry of the space group \mathcal{G} and to compare this symmetry with that of the diagrams in the tables of *IT A*.

With the exception of some double descriptions,⁵ there is exactly one set of diagrams which displays the symmetry of \mathcal{G} , and \mathcal{G} belongs to that space-group type which is described in this set. From those diagrams the Hermann–Mauguin symbol, abbreviated as HM symbol, the Schoenflies symbol and the space-group number are taken.

A rigorous definition is:

Definition 1.2.5.3.1. Two space groups belong to the same *affine space-group type* if and only if they are isomorphic.⁶ \square

This definition refers to a rather abstract property which is of great mathematical but less practical value. In crystallography another definition is more appropriate which results in exactly the same space-group types as are obtained by isomorphism. It starts

⁵ Monoclinic space groups are described in the settings ‘unique axis b ’ and ‘unique axis c ’; rhombohedral space groups are described in the settings ‘hexagonal axes’ and ‘rhombohedral axes’; and 24 space groups are described with two origins by ‘origin choice 1’ and ‘origin choice 2’. In each case, both descriptions lead to the same short Hermann–Mauguin symbol and space-group number.

⁶ The name ‘affine space-group type’ stems from Definition 1.2.5.3.3. ‘Affine space-group types’ have to be distinguished from ‘crystallographic space-group types’ which are defined by Definition 1.2.5.3.4.

from the description of the symmetry operations of a space group by matrix–column pairs or, as will be formulated here, by augmented matrices. For this one refers each of the space groups to one of its lattice bases.

Definition 1.2.5.3.2. Two space groups \mathcal{G} and \mathcal{G}' belong to the same *affine space-group type* if for a lattice basis and an origin of \mathcal{G} , a lattice basis and an origin of \mathcal{G}' can also be found so that the groups of augmented matrices $\{\mathbb{W}\}$ describing \mathcal{G} and $\{\mathbb{W}'\}$ describing \mathcal{G}' are identical. \square

In this definition the coordinate systems are chosen such that the groups of augmented matrices agree. It is thus possible to describe the symmetry of all space groups of the same type by one (standardized) set of matrix–column pairs, as is done, for example, in the tables of *IT A*.

In the subgroup tables of Chapters 2.2 and 2.3 it frequently happens that a subgroup $\mathcal{H} < \mathcal{G}$ of a space group \mathcal{G} is given by its matrix–column pairs referred to a nonconventional coordinate system. In this case, a transformation of the coordinate system can bring the matrix–column pairs to the standard form by which the space-group type may be determined. In the subgroup tables both the space-group type and the transformation of the coordinate system are listed. One can also use this procedure for the definition of the term ‘affine space-group type’:

Definition 1.2.5.3.3. Let two space groups \mathcal{G} and \mathcal{G}' be referred to lattice bases and represented by their groups of augmented matrices $\{\mathbb{W}\}$ and $\{\mathbb{W}'\}$. The groups \mathcal{G} and \mathcal{G}' belong to the same *affine space-group type* if an augmented matrix \mathbb{P} with linear part \mathbf{P} , $\det(\mathbf{P}) \neq 0$, and column part \mathbf{p} exists, for which

$$\{\mathbb{W}'\} = \mathbb{P}^{-1} \{\mathbb{W}\} \mathbb{P} \quad (1.2.5.1)$$

holds. \square

The affine space-group types are classes in the mathematical sense of the word, *i.e.* each space group belongs to exactly one type. The derivation of these types reveals 219 affine space-group types and 17 plane-group types.

In crystallography one usually distinguishes 230 rather than 219 space-group types in a slightly finer subdivision. The difference can best be explained using Definition 1.2.5.3.3. The matrix part \mathbf{P} may have a negative determinant. In this case, a right-handed basis is converted into a left-handed one, and right-handed and left-handed screw axes are exchanged. It is a convention in crystallography to always refer the space to a right-handed basis and hence transformations with $\det(\mathbf{P}) < 0$ are not admitted.

Definition 1.2.5.3.4. If the matrix \mathbf{P} is restricted by the condition $\det(\mathbf{P}) > 0$, 11 affine space-group types split into two space-group types each, one with right-handed and one with left-handed screw axes, such that the total number of types is 230. These 230 space-group types are called *crystallographic space-group types*. The 11 splitting space-group types are called *pairs of enantiomorphic space-group types* and the space groups themselves are enantiomorphic pairs of space groups. \square

The space groups of an enantiomorphic pair belong to different crystallographic space-group types but are isomorphic. As a consequence, in the lists of isomorphic subgroups $\mathcal{H} < \mathcal{G}$ of the tables of Chapter 2.3, there may occur subgroups \mathcal{H} with another conventional HM symbol and another space-group number than that of \mathcal{G} , *cf.* Example 1.2.6.2.7. In such a case, \mathcal{G} and \mathcal{H} are members of an enantiomorphic pair of space groups and \mathcal{H} belongs to the space-group type enantiomorphic to that of \mathcal{G} . There are no enantiomorphic pairs of plane groups.

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The space groups are of different complexity. The simplest ones are the symmorphic space groups (not to be confused with ‘isomorphic’ space groups) according to the following definition:

Definition 1.2.5.3.5. A space group \mathcal{G} is called *symmorphic* if representatives g_k of all cosets $\mathcal{T}(\mathcal{G}) g_k$ can be found such that the set $\{g_k\}$ of all representatives forms a group. \square

The group $\{g_k\}$ is finite and thus leaves a point F fixed. In the standard setting of any symmorphic space group such a point F is chosen as the origin. Thus, the translation parts of the elements g_k consist of zeroes only.

If a space group is symmorphic then all space groups of its type are symmorphic. Therefore, one can speak of ‘symmorphic space-group types’. Symmorphic space groups can be recognized easily by their HM symbols: they contain an unmodified point-group symbol: rotations, reflections, inversions and rotoinversions but no screw rotations or glide reflections. There are 73 symmorphic space-group types of dimension three and 13 of dimension two; none of them show enantiomorphism.

One frequently speaks of ‘the 230 space groups’ or ‘the 17 plane groups’ and does not distinguish between the terms ‘space group’ and ‘space-group type’. This is very often possible and is also done in this volume in order to make the explanations less long-winded. However, occasionally the distinction is indispensable in order to avoid serious difficulties of comprehension. For example, the sentence ‘A space group is a proper subgroup of itself’ is incomprehensible, whereas the sentence ‘A space group and its proper subgroup belong to the same space-group type’ makes sense.

1.2.5.4. Point groups and crystal classes

If the point coordinates are mapped by an isometry and its matrix–column pair, the vector coefficients are mapped by the linear part, *i.e.* by the matrix alone, *cf.* Section 1.2.2.6. Because the number of its elements is infinite, a space group generates from one point an infinite set of symmetry-equivalent points by its matrix–column pairs. Because the number of matrices of the linear parts is finite, the group of matrices generates from one vector a finite set of symmetry-equivalent vectors, *e.g.* the vectors normal to certain planes of the crystal. These planes determine the morphology of the ideal macroscopic crystal and its cleavage; the centre of the crystal represents the zero vector. When the symmetry of a crystal can only be determined by its macroscopic properties, only the symmetry group of the macroscopic crystal can be found. All its symmetry operations leave at least one point of the crystal fixed, *viz* its centre of mass. Therefore, this symmetry group was called the *point group of the crystal*, although its symmetry operations are those of vector space, not of point space. Although misunderstandings are not rare, this name is still used in today’s crystallography for historical reasons.⁷

Let a conventional coordinate system be chosen and the elements $g_j \in \mathcal{G}$ be represented by the matrix–column pairs (W_j, w_j) , with the representation of the translations $t_k \in \mathcal{T}(\mathcal{G})$ by the pairs (I, t_k) . Then the composition of (W_j, w_j) with all translations forms an infinite set $\{(I, t_k)(W_j, w_j) = (W_j, w_j + t_k)\}$ of symmetry operations which is a right coset of the coset decomposition $(\mathcal{G} : \mathcal{T}(\mathcal{G}))$. From this equation it follows that the elements of the same coset of the decomposition $(\mathcal{G} : \mathcal{T}(\mathcal{G}))$ have the same linear part. On the other hand, elements of different cosets have different linear parts if $\mathcal{T}(\mathcal{G})$ contains all translations of \mathcal{G} . Thus, each

coset can be characterized by its linear part. It can be shown from equations (1.2.2.5) and (1.2.2.6) that the linear parts form a group which is isomorphic to the factor group $\mathcal{G}/\mathcal{T}(\mathcal{G})$, *i.e.* to the group of the cosets.

Definition 1.2.5.4.1. A group of linear parts, represented by a group of matrices W_j , is called a *point group* \mathcal{P} . If the linear parts are those of the matrix–column pairs describing the symmetry operations of a space group \mathcal{G} , the group is called the *point group* $\mathcal{P}_{\mathcal{G}}$ of the space group \mathcal{G} . The point groups that can belong to space groups are called *crystallographic point groups*. \square

According to Definition 1.2.5.4.1, the factor group $\mathcal{G}/\mathcal{T}(\mathcal{G})$ is isomorphic to the point group $\mathcal{P}_{\mathcal{G}}$. This property is exploited in the graphs of *translationengleiche* subgroups of space groups, *cf.* Chapter 2.4 and Section 2.1.7.2.

All point groups in the following sections are crystallographic point groups. The maximum order of a crystallographic point group is 48 in three-dimensional space and 12 in two-dimensional space.

As with space groups, there are also an infinite number of crystallographic point groups which may be classified into a finite number of point-group types. This cannot be done by isomorphism because geometrically different point groups may be isomorphic. For example, point groups consisting of the identity with the inversion $\{I, \bar{I}\}$ or with a twofold rotation $\{I, 2\}$ or with a reflection through a plane $\{I, m\}$ are all isomorphic to the (abstract) group of order 2. As for space groups, the classification may be performed, however, referring the point groups to corresponding vector bases. As translations do not occur among the point-group operations, one may choose any basis for the description of the symmetry operations by matrices. One takes the basis of $\{W'\}$ as given and transforms the basis of $\{W\}$ to the basis corresponding to that of $\{W'\}$. This leads to the definition:

Definition 1.2.5.4.2. Two crystallographic point groups $\mathcal{P}_{\mathcal{G}}$ and $\mathcal{P}'_{\mathcal{G}}$ belong to the same *point-group type* or to the same *crystal class of point groups* if there is a real non-singular matrix P which maps a matrix group $\{W\}$ of $\mathcal{P}_{\mathcal{G}}$ onto a matrix group $\{W'\}$ of $\mathcal{P}'_{\mathcal{G}}$ by the transformation $\{W'\} = P^{-1}\{W\}P$. \square

Point groups can be classified by Definition 1.2.5.4.2. Further space groups may be classified into ‘crystal classes of space groups’ according to their point groups:

Definition 1.2.5.4.3. Two space groups belong to the same *crystal class of space groups* if their point groups belong to the same crystal class of point groups. \square

Whether two space groups belong to the same crystal class or not can be worked out from their standard HM symbols: one removes the lattice parts from these symbols as well as the constituents ‘1’ from the symbols of trigonal space groups and replaces all constituents for screw rotations and glide reflections by those for the corresponding pure rotations and reflections. The symbols obtained in this way are those of the corresponding point groups. If they agree, the space groups belong to the same crystal class. The space groups also belong to the same crystal class if the point-group symbols belong to the pair $\bar{4}2m$ and $\bar{4}m2$ or to the pair $\bar{6}2m$ and $\bar{6}m2$.

There are 32 classes of three-dimensional crystallographic point groups and 32 crystal classes of space groups, and ten classes of two-dimensional crystallographic point groups and ten crystal classes of plane groups.

The distribution into crystal classes classifies space-group types – and thus space groups – and crystallographic point groups. It

⁷ The term *point group* is also used for a group of symmetry operations of point space, which is better called a *site-symmetry group* and which is the group describing the symmetry of the surroundings of a point in point space.

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does not classify the infinite set of all lattices into a finite number of lattice types, because the same lattice may belong to space groups of different crystal classes. For example, the same lattice may be that of a space group of type $P1$ (of crystal class 1) and that of a space group of type $P\bar{1}$ (of crystal class $\bar{1}$).

Nevertheless, there is also a definition of the ‘point group of a lattice’. Let a vector lattice \mathbf{L} of a space group \mathcal{G} be referred to a lattice basis. Then the linear parts \mathbf{W} of the matrix–column pairs (\mathbf{W}, \mathbf{w}) of \mathcal{G} form the point group $\mathcal{P}_{\mathcal{G}}$. If (\mathbf{W}, \mathbf{w}) maps the space group \mathcal{G} onto itself, then the linear part \mathbf{W} maps the (vector) lattice \mathbf{L} onto itself. However, there may be additional matrices which also describe symmetry operations of the lattice \mathbf{L} . For example, the point group $\mathcal{P}_{\mathcal{G}}$ of a space group of type $P1$ consists of the identity I only. However, with any vector $\mathbf{t} \in \mathbf{L}$, the negative vector $-\mathbf{t} \in \mathbf{L}$ also belongs to \mathbf{L} . Therefore, the lattice \mathbf{L} is always centrosymmetric and has the inversion $\bar{1}$ as a symmetry operation independent of the symmetry of the space group.

Definition 1.2.5.4.4. The set of all orthogonal mappings with matrices \mathbf{W} which map a lattice \mathbf{L} onto itself is called the point group of the lattice \mathbf{L} or the *holohedry* of the lattice \mathbf{L} . A crystal class of point groups $\mathcal{P}_{\mathcal{G}}$ is called a *holohedral crystal class* if it contains a holohedry. \square

There are seven holohedral crystal classes in the space: $\bar{1}$, $2/m$, mmm , $4/mmm$, $\bar{3}m$, $6/mmm$ and $m\bar{3}m$. Their lattices are called triclinic, monoclinic, orthorhombic, tetragonal, rhombohedral, hexagonal and cubic, respectively. There are four holohedral crystal classes in the plane: 2 , $2mm$, $4mm$ and $6mm$. Their two-dimensional lattices (or nets) are called oblique, rectangular, square and hexagonal, respectively.

The lattices can be classified into *lattice types* or *Bravais types*, mostly called *Bravais lattices*, or into *lattice systems* (called *Bravais systems* in editions 1 to 4 of *IT A*). These classifications are not discussed here because they are not directly relevant to the classification of the space groups. This is because the lattice symmetry is not necessarily typical for the symmetry of its space group but may accidentally be higher. For example, the lattice of a monoclinic crystal may be accidentally orthorhombic (only for certain values of temperature and pressure). In Sections 8.2.5 and 8.2.7 of *IT A* the ‘typical lattice symmetry’ of a space group is defined.

1.2.5.5. Crystal systems and crystal families

The example of $P1$ mentioned above shows that the point group of the lattice may be systematically of higher order than that of its space group. There are obviously point groups and thus space groups that belong to a holohedral crystal class and those that do not. The latter can be assigned to a holohedral crystal class uniquely according to the following definition:⁸

Definition 1.2.5.5.1. A crystal class \mathbf{C} of a space group \mathcal{G} is either holohedral \mathbf{H} or it can be assigned uniquely to \mathbf{H} by the condition: any point group of \mathbf{C} is a subgroup of a point group of \mathbf{H} but not a subgroup of a holohedral crystal class \mathbf{H}' of smaller order. The set of all crystal classes of space groups that are assigned to the same holohedral crystal class is called a *crystal system* of space groups. \square

The 32 crystal classes of space groups are classified into seven crystal systems which are called *triclinic*, *monoclinic*, *orthorhombic*,

bic, *tetragonal*, *trigonal*, *hexagonal* and *cubic*. There are four-crystal systems of plane groups: *oblique*, *rectangular*, *square* and *hexagonal*. Like the space groups, the crystal classes of point groups are classified into the seven crystal systems of point groups.

Apart from accidental lattice symmetries, the space groups of different crystal systems have lattices of different symmetry. As an exception, the hexagonal primitive lattice occurs in both hexagonal and trigonal space groups as the typical lattice. Therefore, the space groups of the trigonal and the hexagonal crystal systems are more related than space groups from other different crystal systems. Indeed, in different crystallographic schools the term ‘crystal system’ was used for different objects. One sense of the term was the ‘crystal system’ as defined above, while another sense of the old term ‘crystal system’ is now called a ‘crystal family’ according to the following definition [for definitions that are also valid in higher-dimensional spaces, see Brown *et al.* (1978) or *IT A*, Chapter 8.2]:

Definition 1.2.5.5.2. In three-dimensional space, the classification of the set of all space groups into crystal families is the same as that into crystal systems with the one exception that the trigonal and hexagonal crystal systems are united to form the *hexagonal crystal family*. There is no difference between crystal systems and crystal families in the plane. \square

The partition of the space groups into crystal families is the most universal one. The space groups and their types, their crystal classes and their crystal systems are classified by the crystal families. Analogously, the crystallographic point groups and their crystal classes and crystal systems are classified by the crystal families of point groups. Lattices, their Bravais types and lattice systems can also be classified into crystal families of lattices; cf. *IT A*, Chapter 8.2.

1.2.6. Types of subgroups of space groups

1.2.6.1. Introductory remarks

Group–subgroup relations form an essential part of the applications of space-group theory. Let \mathcal{G} be a space group and $\mathcal{H} < \mathcal{G}$ a proper subgroup of \mathcal{G} . All maximal subgroups $\mathcal{H} < \mathcal{G}$ of any space group \mathcal{G} are listed in Part 2 of this volume. There are different kinds of subgroups which are defined and described in this section. The tables and graphs of this volume are arranged according to these kinds of subgroups. Moreover, for the different kinds of subgroups different data are listed in the subgroup tables and graphs.

Let \mathcal{G}_j and \mathcal{H}_j be space groups of the space-group types \mathcal{G} and \mathcal{H} . The group–subgroup relation $\mathcal{G}_j > \mathcal{H}_j$ is a relation between the particular space groups \mathcal{G}_j and \mathcal{H}_j but it can be generalized to the space-group types \mathcal{G} and \mathcal{H} . Certainly, not every space group of the type \mathcal{H} will be a subgroup of every space group of the type \mathcal{G} . Nevertheless, the relation $\mathcal{G}_j > \mathcal{H}_j$ holds for any space group of \mathcal{G} and \mathcal{H} in the following sense: If $\mathcal{G}_j > \mathcal{H}_j$ holds for the pair \mathcal{G}_j and \mathcal{H}_j , then for any space group \mathcal{G}_k of the type \mathcal{G} a space group \mathcal{H}_k of the type \mathcal{H} exists for which the corresponding relation $\mathcal{G}_k > \mathcal{H}_k$ holds. Conversely, for any space group \mathcal{H}_m of the type \mathcal{H} a space group \mathcal{G}_m of the type \mathcal{G} exists for which the corresponding relation $\mathcal{G}_m > \mathcal{H}_m$ holds. Only this property of the group–subgroup relations made it possible to compile and arrange the tables of this volume so that they are as concise as those of *IT A*.

1.2.6.2. Definitions and examples

‘Maximal subgroups’ have been introduced by Definition 1.2.4.1.2. The importance of this definition will become apparent

⁸ This assignment does hold for low dimensions of space at least up to dimension 4. A dimension-independent definition of the concepts of ‘crystal system’ and ‘crystal family’ is found in *IT A*, Chapter 8.2, where the classifications are treated in more detail.

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in the corollary to Hermann's theorem, cf. Lemma 1.2.8.1.3. In this volume only the maximal subgroups are listed for any plane and any space group. A maximal subgroup of a plane group is a plane group, a maximal subgroup of a space group is a space group. On the other hand, a minimal supergroup of a plane group or of a space group is not necessarily a plane group or a space group, cf. Section 2.1.6.

If the maximal subgroups are known for each space group, then each non-maximal subgroup of a space group \mathcal{G} with finite index can in principle be obtained from the data on maximal subgroups. A non-maximal subgroup $\mathcal{H} < \mathcal{G}$ of finite index $[i]$ is connected with the original group \mathcal{G} through a chain $\mathcal{H} = \mathcal{Z}_k < \mathcal{Z}_{k-1} < \dots < \mathcal{Z}_1 < \mathcal{Z}_0 = \mathcal{G}$, where each group $\mathcal{Z}_j < \mathcal{Z}_{j-1}$ is a maximal subgroup of \mathcal{Z}_{j-1} , with the index $[i_j] = |\mathcal{Z}_{j-1} : \mathcal{Z}_j|$, $j = 1, \dots, k$. The number k is finite and the relation $i = \prod_{j=1}^k i_j$ holds, i.e. the total index $[i]$ is the product of the indices i_j .

According to Hermann (1929), the following types of subgroups of space groups have to be distinguished:

Definition 1.2.6.2.1. A subgroup \mathcal{H} of a space group \mathcal{G} is called a *translationengleiche subgroup* or a *t-subgroup* of \mathcal{G} if the set $\mathcal{T}(\mathcal{G})$ of translations is retained, i.e. $\mathcal{T}(\mathcal{H}) = \mathcal{T}(\mathcal{G})$, but the number of cosets of $\mathcal{G}/\mathcal{T}(\mathcal{G})$, i.e. the order P of the point group $\mathcal{P}_{\mathcal{G}}$, is reduced such that $|\mathcal{G}/\mathcal{T}(\mathcal{G})| > |\mathcal{H}/\mathcal{T}(\mathcal{H})|$.⁹ □

The order of a crystallographic point group $\mathcal{P}_{\mathcal{G}}$ of the space group \mathcal{G} is always finite. Therefore, the number of the subgroups of $\mathcal{P}_{\mathcal{G}}$ is also always finite and these subgroups and their relations are displayed in well known graphs, cf. Chapter 2.4 and Section 2.1.7 of this volume. Because of the isomorphism between the point group $\mathcal{P}_{\mathcal{G}}$ and the factor group $\mathcal{G}/\mathcal{T}(\mathcal{G})$, the subgroup graph for the point group $\mathcal{P}_{\mathcal{G}}$ is the same as that for the *t*-subgroups of \mathcal{G} , only the labels of the groups are different. For deviations between the point-group graphs and the actual space-group graphs of Chapter 2.4, cf. Section 2.1.7.2.

Example 1.2.6.2.2.

Consider a space group \mathcal{G} of type $P12/m1$ referred to a conventional coordinate system. The translation subgroup $\mathcal{T}(\mathcal{G})$ consists of all translations with translation vectors $\mathbf{t} = u\mathbf{a} + v\mathbf{b} + w\mathbf{c}$, where u, v, w run through all integer numbers. The coset decomposition of $(\mathcal{G} : \mathcal{T}(\mathcal{G}))$ results in the four cosets $\mathcal{T}(\mathcal{G})$, $\mathcal{T}(\mathcal{G})\mathbf{2}_0$, $\mathcal{T}(\mathcal{G})\mathbf{m}_0$ and $\mathcal{T}(\mathcal{G})\bar{\mathbf{I}}_0$, where the right operations are a twofold rotation $\mathbf{2}_0$ around the rotation axis passing through the origin, a reflection \mathbf{m}_0 through a plane containing the origin and an inversion $\bar{\mathbf{I}}_0$ with the inversion point at the origin, respectively. The three combinations $\mathcal{H}_1 = \mathcal{T}(\mathcal{G}) \cup \mathcal{T}(\mathcal{G})\mathbf{2}_0$, $\mathcal{H}_2 = \mathcal{T}(\mathcal{G}) \cup \mathcal{T}(\mathcal{G})\mathbf{m}_0$ and $\mathcal{H}_3 = \mathcal{T}(\mathcal{G}) \cup \mathcal{T}(\mathcal{G})\bar{\mathbf{I}}_0$ each form a *translationengleiche* maximal subgroup of \mathcal{G} of index 2 with the space-group symbols $P121$, $P1m1$ and $P\bar{1}$, respectively.

Definition 1.2.6.2.3. A subgroup $\mathcal{H} < \mathcal{G}$ of a space group \mathcal{G} is called a *klassengleiche subgroup* or a *k-subgroup* if the set $\mathcal{T}(\mathcal{G})$ of all translations of \mathcal{G} is reduced to $\mathcal{T}(\mathcal{H}) < \mathcal{T}(\mathcal{G})$ but all linear parts of \mathcal{G} are retained. Then the number of cosets of the decompositions $\mathcal{H}/\mathcal{T}(\mathcal{H})$ and $\mathcal{G}/\mathcal{T}(\mathcal{G})$ is the same, i.e. $|\mathcal{H}/\mathcal{T}(\mathcal{H})| = |\mathcal{G}/\mathcal{T}(\mathcal{G})|$. In other words: the order of the point group $\mathcal{P}_{\mathcal{H}}$ is the same as that of $\mathcal{P}_{\mathcal{G}}$. See also footnote 9. □

⁹ German: *zellengleiche* means 'with the same cell'; *translationengleiche* means 'with the same translations'; *klassengleiche* means 'of the same (crystal) class'. Of the different German declension endings only the form with terminal *-e* is used in this volume. The terms *zellengleiche* and *klassengleiche* were introduced by Hermann (1929). The term *zellengleiche* was later replaced by *translationengleiche* because of possible misinterpretations. In this volume they are sometimes abbreviated as *t*-subgroups and *k*-subgroups.

For a *klassengleiche* subgroup $\mathcal{H} < \mathcal{G}$, the cosets of the factor group $\mathcal{H}/\mathcal{T}(\mathcal{H})$ are smaller than those of $\mathcal{G}/\mathcal{T}(\mathcal{G})$. Because $\mathcal{T}(\mathcal{H})$ is still infinite, the number of elements of each coset is infinite but the index $|\mathcal{T}(\mathcal{G}) : \mathcal{T}(\mathcal{H})| > 1$ is finite. The number of *k*-subgroups of \mathcal{G} is always infinite.

Example 1.2.6.2.4.

Consider a space group \mathcal{G} of the type $C121$, referred to a conventional coordinate system. The set $\mathcal{T}(\mathcal{G})$ of all translations can be split into the set \mathcal{T}_i of all translations with integer coefficients u, v and w and the set \mathcal{T}_f of all translations for which the coefficients u and v are fractional. The set \mathcal{T}_i forms a group; the set \mathcal{T}_f is the other coset in the decomposition $(\mathcal{T}(\mathcal{G}) : \mathcal{T}_i)$ and does not form a group. Let t_C be the 'centring translation' with the translation vector $\frac{1}{2}(\mathbf{a} + \mathbf{b})$. Then \mathcal{T}_f can be written $\mathcal{T}_i t_C$. Let $\mathbf{2}_0$ mean a twofold rotation around the rotation axis through the origin. There are altogether four cosets of the decomposition $(\mathcal{G} : \mathcal{T}_i)$, which can be written now as \mathcal{T}_i , $\mathcal{T}_f = \mathcal{T}_i t_C$, $\mathcal{T}_i \mathbf{2}_0$ and $\mathcal{T}_f \mathbf{2}_0 = (\mathcal{T}_i t_C) \mathbf{2}_0 = \mathcal{T}_i (t_C \mathbf{2}_0)$. The union $\mathcal{T}_i \cup (\mathcal{T}_i t_C) = \mathcal{T}_{\mathcal{G}}$ forms the *translationengleiche* maximal subgroup $C1$ (conventional setting $P1$) of \mathcal{G} of index 2. The union $\mathcal{T}_i \cup (\mathcal{T}_i \mathbf{2}_0)$ forms the *klassengleiche* maximal subgroup $P121$ of \mathcal{G} of index 2. The union $\mathcal{T}_i \cup (\mathcal{T}_i (t_C \mathbf{2}_0))$ also forms a *klassengleiche* maximal subgroup of index 2. Its HM symbol is $P12_11$, and the twofold rotations $\mathbf{2}$ of the point group $\mathbf{2}$ are realized by screw rotations $\mathbf{2}_1$ in this subgroup because $(t_C \mathbf{2}_0)$ is a screw rotation with its screw axis running parallel to the \mathbf{b} axis through the point $\frac{1}{4}, 0, 0$. There are in fact these two *k*-subgroups of $C121$ of index 2 which have the group \mathcal{T}_i in common. In the subgroup table of $C121$ both are listed under the heading 'Loss of centring translations' because the conventional unit cell is retained while only the centring translations have disappeared. (Four additional *klassengleiche* maximal subgroups of $C121$ are found under the heading 'Enlarged unit cell'.)

The group \mathcal{T}_i of type $P1$ is a non-maximal subgroup of $C121$ of index 4.

Definition 1.2.6.2.5. A *klassengleiche* or *k-subgroup* $\mathcal{H} < \mathcal{G}$ is called *isomorphic* or an *isomorphic subgroup* if it belongs to the same affine space-group type (isomorphism type) as \mathcal{G} . If a subgroup is not isomorphic, it is sometimes called *non-isomorphic*. □

Isomorphic subgroups are special *k*-subgroups. The importance of the distinction between *k*-subgroups in general and isomorphic subgroups in particular stems from the fact that the number of maximal non-isomorphic *k*-subgroups of any space group is finite, whereas the number of maximal isomorphic subgroups is always infinite, see Section 1.2.8.

Example 1.2.6.2.6.

Consider a space group \mathcal{G} of type $P\bar{1}$ referred to a conventional coordinate system. The translation subgroup $\mathcal{T}(\mathcal{G})$ consists of all translations with translation vectors $\mathbf{t} = u\mathbf{a} + v\mathbf{b} + w\mathbf{c}$, where u, v and w run through all integer numbers. There is an inversion $\bar{\mathbf{I}}_0$ with the inversion point at the origin and also an infinite number of other inversions, generated by the combinations of $\bar{\mathbf{I}}_0$ with all translations of $\mathcal{T}(\mathcal{G})$.

We consider the subgroup \mathcal{T}_g of all translations with an even coefficient u and arbitrary integers v and w as well as the coset decomposition $(\mathcal{G} : \mathcal{T}_g)$. Let t_a be the translation with the translation vector \mathbf{a} . There are four cosets: \mathcal{T}_g , $\mathcal{T}_g t_a$, $\mathcal{T}_g \bar{\mathbf{I}}_0$ and $\mathcal{T}_g (t_a \bar{\mathbf{I}}_0)$. The union $\mathcal{T}_g \cup (\mathcal{T}_g t_a)$ forms the *translationengleiche* maximal subgroup $\mathcal{T}(\mathcal{G})$ of index 2. The union $\mathcal{T}_g \cup (\mathcal{T}_g \bar{\mathbf{I}}_0)$ forms an isomorphic maximal subgroup of index 2, as does the

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union $\mathcal{T}_g \cup (\mathcal{T}_g (t_a \bar{I}_0))$. There are thus two maximal isomorphic subgroups of index 2 which are obtained by doubling the a lattice parameter. There are altogether 14 isomorphic subgroups of index 2 for any space group of type $P\bar{1}$ which are obtained by seven different cell enlargements.

If \mathcal{G} belongs to a pair of enantiomorphic space-group types, then the isomorphic subgroups of \mathcal{G} may belong to different crystallographic space-group types with different HM symbols and different space-group numbers. In this case, an infinite number of subgroups belong to the crystallographic space-group type of \mathcal{G} and another infinite number belong to the enantiomorphic space-group type.

Example 1.2.6.2.7.

Space group $P4_1$, No. 76, has for any prime number $p > 2$ an isomorphic maximal subgroup of index p with the lattice parameters a, b, pc . This is an infinite number of subgroups because there is an infinite number of primes. The subgroups belong to the space-group type $P4_1$ if $p \equiv 1 \pmod{4}$; they belong to the type $P4_3$ if $p \equiv 3 \pmod{4}$.

Definition 1.2.6.2.8. A subgroup of a space group is called *general* or a *general subgroup* if it is neither a *translationengleiche* nor a *klassengleiche* subgroup. It has lost translations as well as linear parts, *i.e.* point-group symmetry. \square

Example 1.2.6.2.9.

The subgroup \mathcal{T}_g in Example 1.2.6.2.6 has lost all inversions of the original space group $P\bar{1}$ as well as all translations with odd u . It is a general subgroup $P1$ of the space group $P\bar{1}$ of index 4.

1.2.6.3. The role of normalizers for group–subgroup pairs of space groups

In Section 1.2.4.5, the normalizer $\mathcal{N}_{\mathcal{G}}(\mathcal{H})$ of a subgroup $\mathcal{H} < \mathcal{G}$ in the group \mathcal{G} was defined. The equation $\mathcal{H} \triangleleft \mathcal{N}_{\mathcal{G}}(\mathcal{H}) \leq \mathcal{G}$ holds, *i.e.* \mathcal{H} is a normal subgroup of $\mathcal{N}_{\mathcal{G}}(\mathcal{H})$. The normalizer $\mathcal{N}_{\mathcal{G}}(\mathcal{H})$, by its index in \mathcal{G} , determines the number $N_j = |\mathcal{G} : \mathcal{N}_{\mathcal{G}}(\mathcal{H})|$ of subgroups $\mathcal{H}_j < \mathcal{G}$ that are conjugate in the group \mathcal{G} , *cf.* Remarks (2) and (3) below Definition 1.2.4.5.1.

The group–subgroup relations between space groups become more transparent if one looks at them from a more general point of view. Space groups are part of the general theory of mappings. Particular groups are the *affine group* \mathcal{A} of all reversible affine mappings, the *Euclidean group* \mathcal{E} of all isometries, the *translation group* \mathcal{T} of all translations and the *orthogonal group* \mathcal{O} of all orthogonal mappings.

Connected with any particular space group \mathcal{G} are its group of translations $\mathcal{T}(\mathcal{G})$ and its point group $\mathcal{P}_{\mathcal{G}}$. In addition, the normalizers $\mathcal{N}_{\mathcal{A}}(\mathcal{G})$ of \mathcal{G} in the affine group \mathcal{A} and $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ in the Euclidean group \mathcal{E} are useful. They are listed in Section 15.2.1 of *IT A*. Although consisting of isometries only, $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ is not necessarily a space group, see the paragraph below Lemma 1.2.7.2.6.

For the group–subgroup pairs $\mathcal{H} < \mathcal{G}$ the following relations hold:

$$(1) \quad \mathcal{T}(\mathcal{H}) \leq \mathcal{H} \leq \mathcal{N}_{\mathcal{G}}(\mathcal{H}) \leq \mathcal{G} \leq \mathcal{N}_{\mathcal{E}}(\mathcal{G}) < \mathcal{E};$$

$$(1a) \quad \mathcal{H} \leq \mathcal{N}_{\mathcal{G}}(\mathcal{H}) \leq \mathcal{N}_{\mathcal{E}}(\mathcal{H}) < \mathcal{E};$$

$$(1b) \quad \mathcal{N}_{\mathcal{E}}(\mathcal{H}) \leq \mathcal{N}_{\mathcal{A}}(\mathcal{H}) < \mathcal{A};$$

$$(2) \quad \mathcal{T}(\mathcal{H}) \leq \mathcal{T}(\mathcal{G}) < \mathcal{T} < \mathcal{E};$$

$$(3) \quad \mathcal{T}(\mathcal{G}) \leq \mathcal{G} \leq \mathcal{N}_{\mathcal{E}}(\mathcal{G}) \leq \mathcal{N}_{\mathcal{A}}(\mathcal{G}) < \mathcal{A}.$$

The subgroup \mathcal{H} may be a *translationengleiche* or a *klassengleiche* or a general subgroup of \mathcal{G} . In any case, the normalizer $\mathcal{N}_{\mathcal{G}}(\mathcal{H})$ determines the length of the conjugacy class of $\mathcal{H} < \mathcal{G}$, but it is not feasible to list for each group–subgroup pair $\mathcal{H} < \mathcal{G}$ its normalizer $\mathcal{N}_{\mathcal{G}}(\mathcal{H})$. Indeed, it is only necessary to list for any space group \mathcal{H} its normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{H})$ in the Euclidean group \mathcal{E} of all isometries, as is done in *IT A*, Section 15.2.1. From such a list the normalizers for the group–subgroup pairs can be obtained easily, because for any chain of space groups $\mathcal{H} < \mathcal{G} < \mathcal{E}$, the relations $\mathcal{H} \leq \mathcal{N}_{\mathcal{G}}(\mathcal{H}) \leq \mathcal{G}$ and $\mathcal{H} \leq \mathcal{N}_{\mathcal{G}}(\mathcal{H}) \leq \mathcal{N}_{\mathcal{E}}(\mathcal{H})$ hold. The normalizer $\mathcal{N}_{\mathcal{G}}(\mathcal{H})$ consists consequently of all those isometries of $\mathcal{N}_{\mathcal{E}}(\mathcal{H})$ that are also elements of \mathcal{G} , *i.e.* that belong to the intersection $\mathcal{N}_{\mathcal{E}}(\mathcal{H}) \cap \mathcal{G}$, *cf.* the examples of Section 1.2.7.¹⁰

The isomorphism type of the Euclidean normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{H})$ may depend on the lattice parameters of the space group (*specialized* Euclidean normalizer). For example, if the lattice of the space group $P\bar{1}$ of a triclinic crystal is accidentally monoclinic at a certain temperature and pressure or for a certain composition in a continuous solid-solution series, then the Euclidean normalizer of this space group belongs to the space-group types $P2/m$ or $C2/m$, otherwise it belongs to $P\bar{1}$. Such a *specialized Euclidean normalizer* (here $P2/m$ or $C2/m$) may be distinguished from the *typical Euclidean normalizer* (here $P\bar{1}$), for which the lattice of \mathcal{H} is not more symmetric than is required by the symmetry of \mathcal{H} . The specialized Euclidean normalizers were first listed in the 5th edition of *IT A* (2002), Section 15.2.1.

1.2.7. Application to domain structures

1.2.7.1. Introductory remarks

In this section, the group-theoretical aspects of domain (twin) formation (domain structure, transformation twin) from a homogeneous single crystal (phase **A**, parent phase) to a crystalline phase **B** (daughter phase, deformed phase) are discussed, where the space group \mathcal{H} of phase **B** is a subgroup of the space group \mathcal{G} of phase **A**, $\mathcal{H} < \mathcal{G}$. This happens, *e.g.*, in a displacive or order–disorder phase transition. In most cases phase **B**, the *domain structure*, is inhomogeneous, consisting of homogeneous regions which are called *domains*, defined below.

Only the basic group-theoretical relations are considered here. A deeper discussion of domain structures and their properties needs methods using representation theory, thermodynamic points of view (Landau theory), lattice dynamics and tensor properties of crystals. Such treatments are beyond the scope of this section. A detailed discussion of them is given by Tolédano *et al.* (2003) and by Janovec & Přívratská (2003).

In order to make the group-theoretical treatment possible, the *parent-clamping approximation*, abbreviated PCA, is introduced, by which the lattice parameters of phase **A** are not allowed to change at and after the transition to phase **B**, *cf.* Janovec & Přívratská (2003). Under the assumption of the PCA, two essential conditions hold:

¹⁰ For *maximal* subgroups, a calculation of the conjugacy classes is not necessary because these are indicated in the subgroup tables of Part 2 of this volume by braces to the left of the data sets for the low-index subgroups and by text for the series of isomorphic subgroups. For non-maximal subgroups, the conjugacy relations are not indicated but can be calculated in the way described here. They are also available online on the Bilbao crystallographic server, <http://www.cryst.ehu.es/>, under the program *Subgroupgraph*.

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- (1) The translations of phase **B** are translations of phase **A**. Thus, the space group \mathcal{H} of **B** is a subgroup of the space group \mathcal{G} of **A**, $\mathcal{H} < \mathcal{G}$. Without the PCA, the translations of **B** would not be translations of **A** and, therefore, **H** would not be a subgroup of **G**.
- (2) Under the PCA, the more complicated ferroelastic phases¹¹ display the same simple behaviour as the non-ferroelastic ones. Disturbances which otherwise would be caused in ferroelastic phase transitions do not appear because there is no spontaneous strain.

The domain walls, *i.e.* the boundaries which separate different domains, will not be treated here because their symmetries are layer groups which are two-periodic groups in three-dimensional space and not space groups with three-dimensional periodicity. Layer groups are described in *International Tables for Crystallography*, Vol. E (2002).

Under these assumptions the domains formed may exhibit different chiralities and polarities of their structures and different spatial orientations of their symmetry elements, but each domain has the same specific energy and the lattice of each domain is part of the lattice of the parent structure **A** with space group \mathcal{G} .

In the discussion of domain structures, the following basic concepts are established: domain, domain state, symmetry state, orientation state. These concepts are defined and then applied in different examples of phase transitions in which the group-theoretical procedures and their results are explained.

The second step, the physically realistic situation at a temperature $T_x < T_C$ with the removal of the PCA, is only partly considered in this section. The relaxation of the PCA does not change the relations in a non-ferroelastic phase because all crystal regions suffer the same affine deformation. On the other hand, in ferroelastic phases the different spontaneous strains complicate the relations.

1.2.7.2. Domains, domain states and symmetry states

In a (continuous) phase transition with the symmetry reduction of the space group \mathcal{G} to a subgroup $\mathcal{H} < \mathcal{G}$, a splitting of the parent phase **A** into many crystals of the type **B** is observed. The number of such crystals of **B** is not limited; they differ in their locations in space, in their orientations, in their shapes and in their space groups which, however, all belong to the same space-group type. In order to describe what happens in such a transition, a few notions are useful. If not explicitly stated, the validity of the PCA is assumed.

Definition 1.2.7.2.1. A connected homogeneous part of a domain structure or of a twinned crystal with structure type **B** is called a *domain*. Each domain is a single crystal. The part of the space that is occupied by a domain is the *region* of that domain. \square

If the domains of phase **B** have been formed from a single crystal of phase **A**, then relations between the domains exist which are determined by group theory. In particular, the domains belong to a finite (small) number of domain states which have well defined relations to the original crystal **A** and its space group \mathcal{G} . In order

to describe the relation of **B** to **A**, the notion of crystal pattern is used. Any perfect (ideal) crystal is a finite block of the corresponding infinite arrangement, the symmetry of which is a space group which contains translations. Here, this (infinite) periodic object is called a *crystal pattern*, *cf.* Section 1.2.2.1.

Definition 1.2.7.2.2. Two domains belong to the same *domain state* if their crystal patterns are identical, *i.e.* if they occupy different regions of space that are part of the *same* crystal pattern. In other words: a domain state is a crystal pattern. \square

The number of domain states which are observed after a phase transition is limited and determined by the space groups \mathcal{G} and \mathcal{H} . The number of domains which belong to the same domain state is not limited. The diversity of the domains and their shapes is due to mechanical stresses, defects, electrical charges and nucleation phenomena which strongly influence the kinetics of the phase transition.

A trivial domain structure is formed when phase **B** consists of one domain only, *i.e.* when it forms a *single-domain structure*. This is possible, in particular under an external electric field or under external stress. Such a procedure is known as ‘detwinning’. The corresponding domain state is a *single-domain state*. For a phase transition of the type considered, there are always several single-domain states which have the same *a priori* probability of appearing after a phase transition. In reality not all of them will be observed and/or their relative frequencies and sizes will be rather different.

Single-domain states are introduced in theoretical considerations in order to avoid the complications which may be caused by the coexistence of domains with different spontaneous strain in ferroelastic crystals of the structure **B** if the PCA cannot be assumed. In polydomain structures, the domains would distort or rotate each other a little and thus disturb the simple relations described now. These disturbances do not occur in non-ferroelastic transitions, so for them the simple relations also hold in polydomain structures without the PCA.

Lemma 1.2.7.2.3. The number Z of possible domain states after a phase transition under the PCA is equal to the index i of \mathcal{H} in \mathcal{G} , $Z = |\mathcal{G} : \mathcal{H}| = [i]$. Let $\mathcal{G} = \mathcal{H}_1 \cup \dots \cup g_j \mathcal{H}_1 \cup \dots \cup g_i \mathcal{H}_1$ be the coset decomposition of \mathcal{G} relative to \mathcal{H}_1 , where $g_1 = e, \dots, g_i$ are the coset representatives, and \mathcal{H}_1 is the space group of the domain state **B**₁. The other domain states are obtained from **B**₁ by **B** _{k} = $g_k \mathbf{B}_1$, $k = 2, \dots, i$. For the space group \mathcal{H}_k of the domain state **B** _{k} the following holds: \mathcal{H}_k is obtained by conjugation of the space group \mathcal{H}_1 of **B**₁ with the same element g_k : $\mathcal{H}_k = g_k \mathcal{H}_1 g_k^{-1}$. \square

If in a group–subgroup relation $\mathcal{G} > \mathcal{H}_q$ with index i_q the subgroups \mathcal{H}_q belong to more than one conjugacy class, then each conjugacy class corresponds to a separate phase transition $\mathbf{A} \longrightarrow \mathbf{B}_k^{(1)}$, $\mathbf{A} \longrightarrow \mathbf{B}_k^{(2)}$ etc. These different phase transitions lead to different low-symmetry structures **B**^(m), have different transition temperatures and different probabilities of happening.

There are more elements of the group \mathcal{G} than just g_k that map the domain state **B**₁ onto the domain state **B** _{k} . The elements of the space group \mathcal{H}_1 map the domain state of **B**₁ onto itself: $h_m \mathbf{B}_1 = \mathbf{B}_1$, $h_m \in \mathcal{H}_1$. Therefore, not just the element g_k but all elements $g_k h_m$ of the coset $g_k \mathcal{H}_1$ map the domain state of **B**₁ onto the domain state **B** _{k} : $\mathbf{B}_k = g_k \mathcal{H}_1 \mathbf{B}_1 = g_k \mathbf{B}_1$. This can be expressed in the form:

There is a one-to-one correspondence between the cosets of the decomposition $(\mathcal{G} : \mathcal{H}_1)$ and the possible domain states which may be observed after the transition.

¹¹ A phase transition is called non-ferroelastic if the space groups \mathcal{G} and \mathcal{H} belong to the same crystal family, of which there are six: triclinic, monoclinic, orthorhombic, tetragonal, trigonal–hexagonal and cubic. A phase transition is called ferroelastic if the strain tensor of the low-symmetry phase **B** has more independent components than the strain tensor of the high-symmetry phase **A**. This can only happen if the space groups \mathcal{G} of **A** and \mathcal{H} of **B** belong to different crystal families. In this case, the additional components of the strain tensor of **B** are called *spontaneous strain-tensor components* or *components of the spontaneous deformation*.

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Similarly, all elements $g_k h_m$ map the space group \mathcal{H}_1 onto \mathcal{H}_k by conjugation: $\mathcal{H}_k = g_k h_m \mathcal{H}_1 h_m^{-1} g_k^{-1} = g_k \mathcal{H}_1 g_k^{-1}$.

Note that due to these formulae the i different domain states do not necessarily belong to i different space groups and that *different* domain states may belong to the *same* space group, cf. Lemma 1.2.7.2.6 and Example 1.2.7.2.4.

The terms just defined shall be explained in a few examples. By Example 1.2.7.2.4 a *translationengleiche* transition is displayed; i.e. \mathcal{H} is a *translationengleiche* subgroup of \mathcal{G} . Then the relation between \mathcal{G} and \mathcal{H} is essentially reflected by the relation between the point groups $\mathcal{P}_{\mathcal{G}}$ and $\mathcal{P}_{\mathcal{H}}$.

Example 1.2.7.2.4.

Perovskite BaTiO₃ exhibits a ferroelastic and ferroelectric phase transition from cubic to tetragonal, phase **A** with space group $\mathcal{G} = Pm\bar{3}m$, No. 221, and phase **B**₁ with a *translationengleiche* subgroup $\mathcal{H}_1 = P4mm$, No. 99. Because the index $|\mathcal{G} : \mathcal{H}_1| = 6$, there are six domain states, forming three pairs of domain states which point with their tetragonal c axes along the cubic x , y and z axes of \mathcal{G} . Each pair consists of two antiparallel domain states of opposite polarization (ferroelectric domains). These two domain states belong to the same space group of the type $P4mm$, i.e. the domains of each pair belong to the same symmetry state according to the following definition:

Definition 1.2.7.2.5. Two domains belong to the same *symmetry state* if their space groups are identical. \square

Note that here as in many other places of this section one has to distinguish strictly between ‘space group’ as a specimen, e.g. in ‘space group of a crystal’, and ‘space-group type’, which is one of the 230 classes frequently called simply but inexactly ‘the 230 space groups’, see the last paragraph of Section 1.2.5.3.

Domains of the same domain state always belong to the same symmetry state. Domains of different domain states may or may not belong to the same symmetry state. The number of symmetry states is limited and is smaller than or equal to the number of domain states. Moreover, the number of symmetry states is determined by the space groups \mathcal{G} and \mathcal{H} .

Let $\mathcal{N}_{\mathcal{G}}(\mathcal{H}_1)$ be the normalizer of the space group \mathcal{H}_1 in the space group \mathcal{G} . Then $\mathcal{G} \geq \mathcal{N}_{\mathcal{G}}(\mathcal{H}_1) \supseteq \mathcal{H}_1$ with the indices $|\mathcal{G} : \mathcal{H}_1| = [i]$ and $|\mathcal{G} : \mathcal{N}_{\mathcal{G}}(\mathcal{H}_1)| = [i_N]$ with $i_N \leq i$. By Lemma 1.2.7.2.3, the number $[i] = |\mathcal{G} : \mathcal{H}_1|$ of domain states is determined. For the number of symmetry states the following lemma holds:

Lemma 1.2.7.2.6. The number of symmetry states for the transition **A** \rightarrow **B** with space groups \mathcal{G} and \mathcal{H} is $|\mathcal{G} : \mathcal{N}_{\mathcal{G}}(\mathcal{H})| = i_N \leq i$. To each symmetry state there belong $d_i = i : i_N$ domain states, i.e. $d_i \cdot i_N = i$, cf. Janovec & Přívratská (2003). \square

For the perovskite transition of Example 1.2.7.2.4, the normalizer $\mathcal{N}_{\mathcal{G}}(\mathcal{H}_1)$ can be obtained from the Euclidean normalizer of $P4mm$ in Table 15.2.1.4 of *IT A* which is listed as P^14/mmm . This Euclidean normalizer has continuous translations along the z direction (indicated by the P^1 lattice part of the HM symbol) and is thus not a space group. However, all additional translations of P^14/mmm are not elements of the space group \mathcal{G} , and $\mathcal{N}_{\mathcal{G}}(\mathcal{H}_1) = (\mathcal{N}_{\mathcal{E}}(\mathcal{H}_1) \cap \mathcal{G}) = (P^14/mmm \cap Pm\bar{3}m) = P4/mmm$ is a subgroup of $Pm\bar{3}m$ with index 3 and with the lattice of $Pm\bar{3}m$. Because of the index 3 of $\mathcal{N}_{\mathcal{G}}(\mathcal{H}_1)$ in \mathcal{G} , there are three conjugate subgroups of the type $P4mm$ with their fourfold axes directed along the z , x and y directions of the cubic space group \mathcal{G} . The group \mathcal{H}_1 is a subgroup of index 2 of $\mathcal{N}_{\mathcal{G}}(\mathcal{H}_1)$. Therefore, two domain states (with opposite polar axes)

belong to each of the subgroups \mathcal{H}_j of the space-group type $P4mm$.

In reality, i.e. without the PCA, the additional degree of freedom c/a in tetragonal space groups leads to a metrical inequivalence of the directions of the fourfold axis and the axes perpendicular to it, due to the spontaneous strain. If this ‘true physical situation’ is considered, the 90° angles between the fourfold axes of the domains of different pairs will change slightly because of the ferroelastic tetragonal deformation with subsequent small rotations of the domains. The antiparallel nature of each of the three domain pairs, however, is preserved because they exhibit the same symmetry state, i.e. belong to the same space group.

The space groups \mathcal{G} and \mathcal{H} in the phase transition in perovskites, cf. Example 1.2.7.2.4, are *translationengleiche*. Therefore, $\mathcal{T}(\mathcal{G}) = \mathcal{T}(\mathcal{H})$, and the coset decomposition $(\mathcal{G} : \mathcal{H})$ of the space groups corresponds to the coset decomposition $(\mathcal{P}_{\mathcal{G}} : \mathcal{P}_{\mathcal{H}})$ of their point groups, cf. Section 1.2.6.2. Indeed, in the literature the perovskite transition is nearly always treated using point groups. Other than the *microscopic description* by space groups, the description by point groups is called the *macroscopic* or *continuum description*. Because there are no translations involved, the continuum approach does not require the PCA at all; the point group $4mm$ is for any translations of phase **B** a subgroup of the point group $m\bar{3}m$. However, the spontaneous strains will appear in this ferroelastic transition and will cause the complications mentioned at the end of Section 1.2.7.1 and in the paragraph preceding Lemma 1.2.7.2.3. For non-ferroelastic *translationengleiche* transitions, the application of point groups and of space groups yields equivalent results.

Example 1.2.7.2.4 presents an opportunity to mention another feature of this phase transition which, however, will not be discussed further. The group \mathcal{H}_1 is not a maximal subgroup of \mathcal{G} but $\mathcal{G} > \mathcal{Z}_1 > \mathcal{H}_1$ with $\mathcal{Z}_1 = P4/mmm$ of index 3 in $\mathcal{G} = m\bar{3}m$ and \mathcal{H}_1 of index 2 in \mathcal{Z}_1 . Such ‘intermediate’ domain states between **A** and **B**, like the domain state with the space group \mathcal{Z}_1 , are called *secondary domain states* for thermodynamic reasons. They do not appear in the transition but \mathcal{Z}_1 is the symmetry of the spontaneous strain in the domain state with space group \mathcal{H}_1 . Accidentally, in the present example $\mathcal{Z}_1 = \mathcal{N}_{\mathcal{G}}(\mathcal{H}_1)$ holds. Secondary domain states are treated by Janovec & Přívratská (2003).

1.2.7.3. Translational domain structures (translation twins)

In Example 1.2.7.2.4, a phase transition was discussed which involves only *translationengleiche* group–subgroup relations and, hence, only orientational relations between the domains. The following two examples treat *klassengleiche* transitions, i.e. \mathcal{H} is a *klassengleiche* subgroup of \mathcal{G} , and *translational domain structures*, also called *translation twins*, may appear.

Translational domain structures consist of domains which are parallel, i.e. have the same orientation of their structures (and thus of their lattices) but differ in their location because of the loss of translations of the parent phase in the phase transition. The origins of the larger unit cells of the phase **B** with subgroup \mathcal{H} may coincide with any of the origins of the smaller unit cells of the parent structure **A** with space group \mathcal{G} . Again the number of such domain states is equal to the index of \mathcal{H} in \mathcal{G} , $[i] = |\mathcal{G} : \mathcal{H}|$; the number of symmetry states is $[i_N] = |\mathcal{G} : \mathcal{N}_{\mathcal{G}}(\mathcal{H})|$.

Example 1.2.7.3.1.

Let $\mathcal{G} = Fm\bar{3}m$, No. 225, with lattice parameter a and $\mathcal{H} = Pm\bar{3}m$, No. 221, with the same lattice parameter a . The relation $\mathcal{H} < \mathcal{G}$ is of index 4 and is found between the disordered and ordered modifications of the alloy AuCu₃. In the disor-

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dered state, one Au and three Cu atoms occupy the positions of a cubic F -lattice statistically; in the ordered compound the Au atoms occupy the positions of a cubic P -lattice whereas the Cu atoms occupy the centres of all faces of this cube. According to *IT A*, Table 15.2.1.4, the Euclidean normalizer of \mathcal{H} is $\mathcal{N}_{\mathcal{E}}(\mathcal{H}) = Im\bar{3}m$ with lattice parameter a . The additional I centring translations of $\mathcal{N}_{\mathcal{E}}(\mathcal{H})$ are not translations of \mathcal{G} and thus $\mathcal{N}_{\mathcal{G}}(\mathcal{H}) = \mathcal{H}$. There are four domain states, each one with its own distinct space group and symmetry state \mathcal{H}_j , $j = 1, \dots, 4$, and consequently its own conventional origin relative to the origin of the disordered crystal \mathbf{A} with the space group \mathcal{G} . The origin shifts of \mathbf{B}_j relative to the origin of \mathbf{A} are $0, 0, 0$; $\frac{1}{2}, \frac{1}{2}, 0$; $\frac{1}{2}, 0, \frac{1}{2}$ and $0, \frac{1}{2}, \frac{1}{2}$.

These shifts do not show up in the macroscopic properties of the domains. Indeed, one is normally neither interested in those translations of \mathcal{G} which are lost in the transition to the subgroup \mathcal{H} , nor in the position of the conventional origin of \mathbf{B} relative to that of \mathbf{A} but only in the orientation of the domain states \mathbf{B}_k . If so, the observed relations are not governed by the space groups \mathcal{G} and \mathcal{H} but by \mathcal{G} and Hermann's group \mathcal{M} , $\mathcal{G} \geq \mathcal{M} \geq \mathcal{H}$, cf. Lemma 1.2.8.1.2. The group \mathcal{M} is uniquely determined as the space group with the translations of \mathcal{G} and the point-group operations of \mathcal{H} . The group \mathcal{M} can thus be characterized as that *translationengleiche* subgroup of \mathcal{G} which is at the same time a *klassengleiche* supergroup of \mathcal{H} . This group \mathcal{M} plays a role in the practical treatment of domains. It was applied to domain structures first by Janovec (1976).

In the current literature, the following considerations are mostly restricted to the point groups of the phases involved. In the following, the use of Hermann's group \mathcal{M} is discussed in parallel with the normal use of the point groups. The (admittedly rather abstract) discussion may thus be unfamiliar to the reader. Nevertheless, it is offered here because it opens up the possibility of treating phase transitions on a microscopic or atomistic level, whereas the point-group approach can only deal with the continuum or macroscopic aspect. The microscopic approach is necessary in particular when discussing domain boundaries, which will not be done here.

Definition 1.2.7.3.2. Two domain states \mathbf{B}_1 and \mathbf{B}_k with space groups \mathcal{H}_1 and \mathcal{H}_k and point groups $\mathcal{P}_{\mathcal{H}_1}$ and $\mathcal{P}_{\mathcal{H}_k}$ have the *same orientation state* if their orientation is identical, *i.e.* if the linear part of the operation $g_k \in \mathcal{G}$ of Lemma 1.2.7.2.3 is the identity operation. This means that $g_k \in \mathcal{G}$ is a translation $t \in \mathcal{T}$ and implies that the point groups of \mathbf{B}_1 and \mathbf{B}_k are the same: $\mathcal{P}_{\mathcal{H}_1} = \mathcal{P}_{\mathcal{H}_k}$. Thus the space groups \mathcal{H}_1 and \mathcal{H}_k are subgroups of the same space group \mathcal{M} . \square

Lemma 1.2.7.3.3. The number of orientation states in the transition $\mathbf{A} \rightarrow \mathbf{B}$ with space groups $\mathcal{G} \rightarrow \mathcal{H}_m$ is $|\mathcal{G} : \mathcal{M}_m|$, *i.e.* the index of \mathcal{M}_m in \mathcal{G} , where \mathcal{M}_m is Hermann's group in the sequence $\mathcal{G} \geq \mathcal{M}_m \geq \mathcal{H}_m$. These orientation states belong to $|\mathcal{G} : \mathcal{N}_{\mathcal{G}}(\mathcal{M}_m)|$ space groups. The number of domain states which belong to the same orientation state is $|\mathcal{M}_m : \mathcal{H}_m|$, *i.e.* the index of \mathcal{H}_m in \mathcal{M}_m . \square

In Example 1.2.7.3.1 of AuCu_3 , $\mathcal{G} = \mathcal{M}_1$ because \mathcal{H}_1 is a *klassengleiche* subgroup of \mathcal{G} . Therefore, $|\mathcal{G} : \mathcal{M}_1| = 1$ and all four domain states belong to the same orientation state. This is obvious visually, because, as stated above, all four domain states are parallel and only shifted against each other.

Lemma 1.2.7.3.4. Because of the isomorphism $(\mathcal{G} : \mathcal{M}) \cong (\mathcal{P}_{\mathcal{G}} : \mathcal{P}_{\mathcal{H}})$ between the factor groups $(\mathcal{G} : \mathcal{M})$ and $(\mathcal{P}_{\mathcal{G}} : \mathcal{P}_{\mathcal{H}})$, the

results of the application of the groups \mathcal{G} and \mathcal{M} are the same as the results of the application of the groups $\mathcal{P}_{\mathcal{G}}$ and $\mathcal{P}_{\mathcal{H}}$. The latter application is called the 'continuum approach to phase transitions' which is nearly always applied in practice. \square

Lemma 1.2.7.3.3 is the microscopic formulation of the (macroscopic) continuum treatment of phase transitions and forms the bridge from the (macroscopic) continuum to the (microscopic) atomistic approach to phase transitions.

Example 1.2.7.3.5.

There is an order-disorder transition of the alloy β -brass, CuZn . In the disordered state the Cu and Zn atoms occupy statistically the positions of a cubic I lattice with space group $\mathcal{G} = Im\bar{3}m$, No. 229. In the ordered state, both kinds of atoms form a cubic primitive lattice P each, and one kind of atom occupies the centres of the cubes of the other, such that a space group $Pm\bar{3}m$, No. 221, is formed, see also Example 1.3.3.1. For the space groups the relation $\mathcal{G} = Im\bar{3}m > \mathcal{H} = Pm\bar{3}m$ of index 2 holds with the same cubic lattice parameter a . In this case, $\mathcal{G} = \mathcal{N}_{\mathcal{E}}(\mathcal{H})$, see *IT A*, Table 15.2.1.4. As the index $|\mathcal{G} : \mathcal{H}| = 2$, there are two domain states with their crystal structures shifted relative to each other by $\frac{1}{2}(\mathbf{a} + \mathbf{b} + \mathbf{c})$. Thus, both domain states belong to the same orientation state. This also follows from $\mathcal{G} = \mathcal{M}$. Because $\mathcal{G} = \mathcal{N}_{\mathcal{G}}(\mathcal{H})$ and thus $|\mathcal{G} : \mathcal{N}_{\mathcal{G}}(\mathcal{H})| = 1$, there is one symmetry state, and both domain states belong to the same space group.

1.2.7.4. Domain structures of a general phase transition

Up to now, the examples have been concerned either with *translationengleiche* or with *klassengleiche* transitions only. In this section, the domain structure of a *general* transition will be considered, *i.e.* a transition where \mathcal{H} is a general subgroup of \mathcal{G} . General subgroups are not listed in this volume but have to be derived from the maximal subgroups of each single step of the group-subgroup chain between \mathcal{G} and \mathcal{H} . In the following Example 1.2.7.4.2, the chain has two steps. The results obtained under the PCA and without it are different and, therefore, will be discussed in some detail. Example 1.2.7.4.2 further shows how the subgroup data of this volume can be used for the analysis of continuous or quasi-continuous phase transitions.

We start with a lemma for general subgroups which contains the results of Lemmata 1.2.7.3.3 and 1.2.7.3.4.

Lemma 1.2.7.4.1. For general subgroups, owing to the existence of the group \mathcal{M} of Hermann, it always holds that $|\mathcal{G} : \mathcal{H}| = |\mathcal{G} : \mathcal{M}| \cdot |\mathcal{M} : \mathcal{H}| = |\mathcal{P}_{\mathcal{G}} : \mathcal{P}_{\mathcal{H}}| \cdot |\mathcal{I}(\mathcal{G}) : \mathcal{I}(\mathcal{H})| = i_P \cdot i_T$. Here i_P is the index of the point groups of \mathcal{G} and \mathcal{H} and i_T is the index of the translation subgroups of \mathcal{G} and \mathcal{H} . \square

Example 1.2.7.4.2.

β -Gadolinium molybdate, $\text{Gd}_2(\text{MoO}_4)_3$, is ferroelectric and ferroelastic. The high-temperature phase \mathbf{A} has space group $\mathcal{G} = P\bar{4}2_1m$, No. 113, and basis vectors \mathbf{a} , \mathbf{b} and \mathbf{c} . At $T_C \sim 433$ K, a phase transition to a low-temperature phase \mathbf{B} occurs with space-group type $\mathcal{H} = Pba2$, No. 32, basis vectors $\mathbf{a}' = \mathbf{a} - \mathbf{b}$, $\mathbf{b}' = \mathbf{a} + \mathbf{b}$ and $\mathbf{c}' = \mathbf{c}$. The group \mathcal{M} , $\mathcal{G} > \mathcal{M} > \mathcal{H}$ is of the type $Cmm2$ with the lattice parameters of \mathcal{H} . The index of \mathcal{H} in \mathcal{G} is $i = |P\bar{4}2_1m : Pba2| = 4$. A factor of 2 stems from the reduction $i_P = |\mathcal{G} : \mathcal{M}| = 2$ and leads to two orientation states. The other factor of 2 is caused by the loss of half of the translations, because $i_T = |\mathcal{M} : \mathcal{H}| = 2$.

In the continuum description, we consider the point groups and $|\bar{4}2m : mm2| = 2$. There is only one subgroup of $\bar{4}2m$ of the type $mm2$. Thus, the two orientation states belong to the same

point group. The orientation state \mathbf{B}_2 is obtained from \mathbf{B}_1 by the (lost) $\bar{4}$ operation of $\bar{4}2m$.

This is the *macroscopic* or *continuum treatment*; it is the most common treatment of domains in phase transitions. In reality, *i.e.* lifting the PCA, due to the orthorhombic symmetry of phase \mathbf{B} the domains will be slightly distorted and rotated, and thus the symmetry planes of the two domain states are no longer parallel.

The full microscopic or atomistic treatment has to consider the crystal structures of phases \mathbf{A} and \mathbf{B} . Under the PCA, the length of a' and b' is $(2)^{1/2}a$, the content of the unit cell of \mathbf{B}_1 is twice that of \mathbf{A} . Because the index $[i] = 4$ there are four domain states \mathbf{B}_1 to \mathbf{B}_4 of $Pba2$. The domain state \mathbf{B}_2 is obtained from \mathbf{B}_1 by the (lost) $\bar{4}$ operation of $P\bar{4}2_1m$. The same holds for the pair \mathbf{B}_3 and \mathbf{B}_4 . Thus, \mathbf{B}_2 & \mathbf{B}_4 are rotated by 90° around a $\bar{4}$ centre in the $(a' b')$ plane with respect to the pair \mathbf{B}_1 & \mathbf{B}_3 , and the c' axes are antiparallel for \mathbf{B}_2 & \mathbf{B}_4 relative to those of \mathbf{B}_1 & \mathbf{B}_3 . The orientation state of the pair \mathbf{B}_1 & \mathbf{B}_3 is different from that of \mathbf{B}_2 & \mathbf{B}_4 . The two pairs \mathbf{B}_1 & \mathbf{B}_2 and \mathbf{B}_3 & \mathbf{B}_4 are shifted relative to each other by a (lost) translation of $P\bar{4}2_1m$, *e.g.* by $t(1, 0, 0)$ in the basis of $P\bar{4}2_1m$, corresponding to $t(\frac{1}{2}, \frac{1}{2}, 0)$ in the basis of $Pba2$.

To calculate the number of space groups $Pba2$, *i.e.* the number of symmetry states, one determines the normalizer of $Pba2$ in $P\bar{4}2_1m$. From IT A, Table 15.2.1.3, one finds $\mathcal{N}_{\mathcal{E}}(Pba2) = P^14/mmm$ for the Euclidean normalizer of $Pba2$ under the PCA, which includes the condition $a = b$. P^14/mmm is a supergroup of $P\bar{4}2_1m$. Thus, $\mathcal{N}_{\mathcal{G}}(Pba2) = (\mathcal{N}_{\mathcal{E}}(Pba2) \cap \mathcal{G}) = \mathcal{G}$ and $|\mathcal{G} : \mathcal{N}_{\mathcal{G}}(Pba2)| = |\mathcal{G} : \mathcal{G}| = 1$. Therefore, under the PCA all four domain states belong to one symmetry state, *i.e.* to one space group $Pba2$.

Analysing the group–subgroup relations between $P\bar{4}2_1m$ and $Pba2$ with the tables of this volume, one finds only one chain $P\bar{4}2_1m \rightarrow Cmm2 \rightarrow Pba2$. For $P\bar{4}2_1m$ only one maximal subgroup of type $Cmm2$ is listed, for which again only one maximal subgroup of type $Pba2$ is found, in agreement with the previous paragraph.

In reality, *i.e.* relaxing the PCA, the observations are made at temperatures $T_x < T_C$ where the lattice parameters deviate from those of phase \mathbf{A} and the basis no longer has tetragonal symmetry, but orthorhombic symmetry, $a' < b'$. The previous single space group now splits into *two* different space groups of type $Pba2$ with orthorhombic metrics at T_x , one belonging to the pair \mathbf{B}_1 & \mathbf{B}_3 , the other to \mathbf{B}_2 & \mathbf{B}_4 . The $(\mathbf{a}', \mathbf{b}')$ bases of these pairs are oriented perpendicular to each other and the c' axes of their domains are antiparallel. The loss of the centring translation of $Cmm2$ does not produce a new space group.

The number, two, of these space groups if the PCA is not valid can also be calculated in the usual way with the help of the normalizer. The Euclidean normalizer of $Pba2$ with $a' \neq b'$ is $\mathcal{N}_{\mathcal{E}}(Pba2) = P^1mmm$. This is an orthorhombic group with continuous translations along the c' direction. P^1mmm with $a' \neq b'$ is not really a subgroup of $P\bar{4}2_1m$ because the translations of $Pba2$ and thus of $Cmm2$ and P^1mmm are not strictly translations of $P\bar{4}2_1m$. The first three groups have orthorhombic lattices and the last a tetragonal one. However, by relaxing the PCA only gradually, the difference between the orthorhombic groups and the corresponding groups with tetragonal lattices is arbitrarily small. Therefore, one considers the sequence $\mathcal{G} > \mathcal{M} = \mathcal{N}_{\mathcal{G}}(\mathcal{H}) > \mathcal{H}$, *i.e.* $P\bar{4}2_1m > Cmm2 > Pba2$ as a group–subgroup chain, forms the intersection $(P^1mmm \cap P\bar{4}2_1m)$ as if the groups would have common translations, and finds $\mathcal{N}_{\mathcal{G}}(\mathcal{H}) = Cmm2$ with approxi-

mately the lattice parameters of $P\bar{4}2_1m$. The index $|P\bar{4}2_1m : Cmm2| = 2$, such that there are two space groups of type $Pba2$ which are approximately subgroups of $P\bar{4}2_1m$. To each of these space groups $Pba2$ belong two domain states of phase \mathbf{B} , see above.

This example shows that without the PCA, in order to cope with real observations, the terms ‘subgroup’, ‘intersection of groups’ *etc.* must not be used *sensu stricto* but have to be relaxed. The orthorhombic translations in this example are not group elements of \mathcal{G} but are slightly modified from the original translations of \mathcal{G} . All group–subgroup relations in crystal chemistry, *e.g.* diamond (C)–sphalerite (ZnS), as well as many phase transitions, as in this example, require such a ‘softened’ approach.

It turns out that the transition of $Gd_2(MoO_4)_3$ can be considered both under the PCA (allowing exact group-theoretical arguments) and under physically realistic arguments (which require certain relaxations of the group-theoretical methods). The results are different but the realistic approach can be developed by means of an increasing deviation from the PCA, starting from idealized but unrealistic considerations.

1.2.8. Lemmata on subgroups of space groups

There are several lemmata on subgroups $\mathcal{H} < \mathcal{G}$ of space groups \mathcal{G} which may help in getting an insight into the laws governing group–subgroup relations of plane and space groups. They were also used for the derivation and the checking of the tables of Part 2. These lemmata are proved or at least stated and explained in Chapter 1.5. They are repeated here as statements, separated from their mathematical background, and are formulated for the three-dimensional space groups. They are valid by analogy for the (two-dimensional) plane groups.

1.2.8.1. General lemmata

Lemma 1.2.8.1.1. A subgroup \mathcal{H} of a space group \mathcal{G} is a space group again, if and only if the index $i = |\mathcal{G} : \mathcal{H}|$ is finite. \square

In this volume, only subgroups of finite index i are listed. However, the index i is not restricted, *i.e.* there is no number I with the property $i < I$ for any i . Subgroups $\mathcal{H} < \mathcal{G}$ with infinite index are considered in *International Tables for Crystallography*, Vol. E (2002).

Lemma 1.2.8.1.2. Hermann’s theorem. For any group–subgroup chain $\mathcal{G} > \mathcal{H}$ between space groups there exists a uniquely defined space group \mathcal{M} with $\mathcal{G} \geq \mathcal{M} \geq \mathcal{H}$, where \mathcal{M} is a *translationengleiche* subgroup of \mathcal{G} and \mathcal{H} is a *klassengleiche* subgroup of \mathcal{M} . \square

The decisive point is that any group–subgroup chain between space groups can be split into a *translationengleiche* subgroup chain between the space groups \mathcal{G} and \mathcal{M} and a *klassengleiche* subgroup chain between the space groups \mathcal{M} and \mathcal{H} .

It may happen that either $\mathcal{G} = \mathcal{M}$ or $\mathcal{H} = \mathcal{M}$ holds. In particular, one of these equations must hold if $\mathcal{H} < \mathcal{G}$ is a maximal subgroup of \mathcal{G} .

Lemma 1.2.8.1.3. (Corollary to Hermann’s theorem.) A maximal subgroup of a space group is either a *translationengleiche* subgroup or a *klassengleiche* subgroup, never a general subgroup. \square

The following lemma holds for space groups but not for arbitrary groups of infinite order.

Lemma 1.2.8.1.4. For any space group, the number of subgroups with a given finite index i is *finite*. \square

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This number of subgroups can be further specified, see Chapter 1.5. Although for each index i the number of subgroups is finite, the number of all subgroups with finite index is infinite because there is no upper limit for the number i .

1.2.8.2. Lemmata on maximal subgroups

Even the set of all *maximal* subgroups of finite index is not finite, as can be seen from the following lemma.

Lemma 1.2.8.2.1. The index i of a maximal subgroup of a space group is always of the form p^n , where p is a prime number and $n = 1$ or 2 for plane groups and $n = 1, 2$ or 3 for space groups. \square

An index of p^2 , $p > 2$, occurs only for isomorphic subgroups of tetragonal, trigonal and hexagonal space groups when the basis vectors are enlarged to $p\mathbf{a}$, $p\mathbf{b}$. An index of p^3 occurs for and only for isomorphic subgroups of cubic space groups with cell enlargements of $p\mathbf{a}$, $p\mathbf{b}$, $p\mathbf{c}$ ($p > 2$).

This lemma means that a subgroup of, say, index 6 cannot be maximal. Moreover, because of the infinite number of primes, the set of all maximal subgroups of a given space group cannot be finite.

There are even stronger restrictions for *maximal non-isomorphic* subgroups.

Lemma 1.2.8.2.2. The index of a maximal non-isomorphic subgroup of a plane group is 2 or 3; for a space group the index is 2, 3 or 4. \square

This lemma can be specified further:

Lemma 1.2.8.2.3. The index of a maximal non-isomorphic subgroup \mathcal{H} is always 2 for oblique, rectangular and square plane groups and for triclinic, monoclinic, orthorhombic and tetragonal

space groups \mathcal{G} . The index is 2 or 3 for hexagonal plane groups and for trigonal and hexagonal space groups \mathcal{G} . The index is 2, 3 or 4 for cubic space groups \mathcal{G} . \square

There are also lemmata for the number of subgroups of a certain index. The most important are:

Lemma 1.2.8.2.4. The number of subgroups of index 2 is $2^N - 1$ with $0 \leq N \leq 6$ for space groups and $0 \leq N \leq 4$ for plane groups. The number of *translationengleiche* subgroups of index 2 is $2^M - 1$ with $0 \leq M \leq 3$ for space groups and $0 \leq M \leq 2$ for plane groups. \square

Examples are:

$N = 0$: $2^0 - 1 = 0$ subgroups of index 2 for $p3$, No. 13, and

$F23$, No. 196;

$N = 1$: $2^1 - 1 = 1$ subgroup of index 2 for $p3m1$, No. 14, and

$P3$, No. 143; ... ;

$N = 4$: $2^4 - 1 = 15$ subgroups of index 2 for $p2mm$, No. 6,

and $P\bar{1}$, No. 2;

$N = 6$: $2^6 - 1 = 63$ subgroups of index 2 for $Pmmm$, No. 47.

Lemma 1.2.8.2.5. The number of isomorphic subgroups of each space group is infinite and this applies even to the number of maximal isomorphic subgroups. \square

Nevertheless, their listing is possible in the form of infinite series. The series are specified by parameters.

Lemma 1.2.8.2.6. For each space group, each maximal isomorphic subgroup \mathcal{H} can be listed as a member of one of at most four series of maximal isomorphic subgroups. Each member is specified by a set of parameters. \square

The series of maximal isomorphic subgroups are discussed in Section 2.1.5.

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