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8.1. Basic concepts

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8.1.1. Introduction

The aim of this part is to define and explain some of the concepts and terms frequently used in crystallography, and to present some basic knowledge in order to enable the reader to make best use of the space-group tables.

The reader will be assumed to have some familiarity with analytical geometry and linear algebra, including vector and matrix calculus. Even though one can solve a good number of practical crystallographic problems without this knowledge, some mathematical insight is necessary for a more thorough understanding of crystallography. In particular, the application of symmetry theory to problems in crystal chemistry and crystal physics requires a background of group theory and, sometimes, also of representation theory.

The symmetry of crystals is treated in textbooks by different methods and at different levels of complexity. In this part, a mainly algebraic approach is used, but the geometric viewpoint is presented also. The algebraic approach has two advantages: it facilitates computer applications and it permits statements to be formulated in such a way that they are independent of the dimension of the space. This is frequently done in this part.

A great selection of textbooks and monographs is available for the study of crystallography. Only Giacovazzo (2002) and Vainshtein (1994) will be mentioned here.

Surveys of the history of crystallographic symmetry can be found in Burckhardt (1988) and Lima-de-Faria (1990).

In addition to books, many programs exist by which crystallographic computations can be performed. For example, the programs can be used to derive the classes of point groups, space groups, lattices (Bravais lattices) and crystal families; to calculate the subgroups of point groups and space groups, Wyckoff positions, irreducible representations *etc.* The mathematical program packages *GAP* (Groups, Algorithms and Programming), in particular *CrystGap*, and *Carat* (Crystallographic Algorithms and Tables) are examples of powerful tools for the solution of problems of crystallographic symmetry. For *GAP*, see http://www.gap-system.org/; for *Carat*, see http://wwwb.math.rwth-aachen.de/carat/. Other programs are provided by the crystallographic server in Bilbao: http://www.cryst.ehu.es/cryst/.

Essential for the determination of crystal structures are extremely efficient program systems that implicitly make use of crystallographic (and noncrystallographic) symmetries.

In this part, as well as in the space-group tables of this volume, 'classical' crystallographic groups in three, two and one dimensions are described, *i.e.* space groups, plane groups, line groups and their associated point groups. In addition to three-dimensional crystallography, which is the basis for the treatment of crystal structures, crystallography of two- and one-dimensional space is of practical importance. It is encountered in sections and projections of crystal structures, in mosaics and in frieze ornaments.

There are several expansions of 'classical' crystallographic groups (groups of motions) that are not treated in this volume but will or may be included in future volumes of the *IT* series.

(*a*) Generalization of crystallographic groups to spaces of dimension $n > 3$ is the field of n-dimensional crystallography. Some results are available. The crystallographic symmetry operations for spaces of any dimension n have already been derived by Hermann (1949). The crystallographic groups of four-dimensional space are also completely known and have been tabulated by Brown *et al.* (1978) and Schwarzenberger (1980). The present state of the art and results for higher dimensions are described by Opgenorth *et al.* (1998), Plesken & Schulz (2000) and Souvignier (2003). Some of their results are displayed in Table 8.1.1.1.

(*b*) One can deal with groups of motions whose lattices of translations have lower dimension than the spaces on which the groups act. This expansion yields the *subperiodic groups*. In particular, there are frieze groups (groups in a plane with one-dimensional translations), rod groups (groups in space with one-dimensional translations) and layer groups (groups in space with two-dimensional translations). These subperiodic groups are treated in *IT* E (2002) in a similar way to that in which line groups, plane groups and space groups are treated in this volume. Subperiodic groups are strongly related to 'groups of generalized symmetry'.

(*c*) Incommensurate phases, *e.g.* modulated structures or inclusion compounds, as well as quasicrystals, have led to an extension of crystallography beyond periodicity. Such structures are not really periodic in three-dimensional space but their symmetry may be described as that of an n-dimensional periodic structure, *i.e.* by an n-dimensional space group. In practical cases, $n = 4$, 5 or 6 holds. The crystal structure is then an irrational three-dimensional section through the n-dimensional periodic structure. The description by crystallographic groups of higher-dimensional spaces is thus of practical interest, *cf.* Janssen *et al.* (2004), van Smaalen (1995) or Yamamoto (1996).

(*d*) Generalized symmetry. Other generalizations of crystallographic symmetry combine the geometric symmetry operations with changes of properties: black–white groups, colour groups *etc.* They are treated in the classical book by Shubnikov & Koptsik (1974). Janner (2001) has given an overview of further generalizations.

8.1.2. Spaces and motions

Crystals are objects in the physical three-dimensional space in which we live. A model for the mathematical treatment of this space is the so-called *point space*, which in crystallography is known as *direct* or *crystal space*. In this space, the structures of finite real crystals are idealized as infinite perfect three-dimensional crystal structures (*cf.* Section 8.1.4). This implies that for crystal structures and their symmetries the surfaces of crystals as well as their defects and imperfections are neglected; for most applications, this is an excellent approximation.

The description of crystal structures and their symmetries is not as simple as it appears at first sight. It is useful to consider not only

Table 8.1.1.1. *Number of crystallographic classes for dimensions 1 to 6*

The numbers are those of the *affine* equivalence classes. The numbers for the enantiomorphic pairs are given in parentheses preceded by a + sign (Souvignier, 2003).

Dimension of space	Crystal families	Lattice (Bravais) types	(Geometric) crystal classes	Arithmetic crystal classes	Space-group types
1	1	1	2	2	2
2	4	5	10	13	17
3	6	14	32	73	(+11) 219
4	(+6) 23	(+10) 64	(+44) 227	(+70) 710	(+111) 4783
5	32	189	955	6079	222018
6	91	841	7104	(+30) 85311	(+7052) 28927922

the above-mentioned point space but also to introduce simultaneously a *vector space* which is closely connected with the point space. Crystallographers are used to working in both spaces: crystal structures are described in point space, whereas face normals, translation vectors, Patterson vectors and reciprocal-lattice vectors are elements of vector spaces.

In order to carry out crystallographic calculations it is necessary to have a *metrics* in point space. Metrical relations, however, are most easily introduced in vector space by defining scalar products between vectors from which the length of a vector and the angle between two vectors are derived. The connection between the vector space $\mathbf{V}^n$ and the point space E^n transfers both the metrics and the dimension of $\mathbf{V}^n$ onto the point space E^n in such a way that distances and angles in point space may be calculated.

The connection between the two spaces is achieved in the following way:

(i) To any two points P and Q of the point space E^n a vector $\overrightarrow{PQ} = \mathbf{r}$ of the vector space $\mathbf{V}^n$ is attached.

(ii) For each point P of E^n and each vector $\mathbf{r}$ of $\mathbf{V}^n$ there is exactly one point Q of E^n for which $\overrightarrow{PQ} = \mathbf{r}$ holds.

(iii) $\overrightarrow{PQ} + \overrightarrow{QR} = \overrightarrow{PR}$.

The distance between two points P and Q in point space is given by the length $|\overrightarrow{PQ}| = (\overrightarrow{PQ}, \overrightarrow{PQ})^{1/2}$ of the attached vector $\overrightarrow{PQ}$ in vector space. In this expression, $(\overrightarrow{PQ}, \overrightarrow{PQ})$ is the scalar product of $\overrightarrow{PQ}$ with itself.

The angle determined by P, Q and R with vertex Q is obtained from

$$\cos(P,Q,R) = \cos(\overrightarrow{QP}, \overrightarrow{QR}) = \frac{(\overrightarrow{QP}, \overrightarrow{QR})}{|\overrightarrow{QP}| \cdot |\overrightarrow{QR}|}.$$

Here, $(\overrightarrow{QP}, \overrightarrow{QR})$ is the scalar product between $\overrightarrow{QP}$ and $\overrightarrow{QR}$. Such a point space is called an n-dimensional *Euclidean space*.

If we select in the point space E^n an arbitrary point O as the *origin*, then to each point X of E^n a unique vector $\overrightarrow{OX}$ of $\mathbf{V}^n$ is assigned, and there is a one-to-one correspondence between the points X of E^n and the vectors $\overrightarrow{OX}$ of $\mathbf{V}^n : X \leftrightarrow \overrightarrow{OX} = \mathbf{x}$.

Referred to a vector basis $\mathbf{a}_1, \ldots, \mathbf{a}_n$ of $\mathbf{V}^n$, each vector $\mathbf{x}$ is uniquely expressed as $\mathbf{x} = x_1\mathbf{a}_1 + \ldots + x_n\mathbf{a}_n$ or, using matrix multiplication,* $\mathbf{x} = (\mathbf{a}_1, \ldots, \mathbf{a}_n)\begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix}$.

Referred to the coordinate system $(O, \mathbf{a}_1, \ldots, \mathbf{a}_n)$ of E^n, Fig. 8.1.2.1, each point X is uniquely described by the column of coordinates

$$\boldsymbol{x} = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix}.$$

Thus, the real numbers x_i are either the *coefficients of the vector* $\mathbf{x}$ of $\mathbf{V}^n$ or the *coordinates of the point* X of E^n.

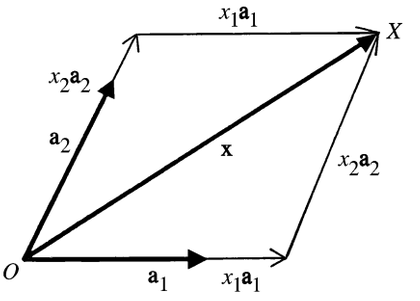

Fig. 8.1.2.1. Representation of the point X with respect to origin O by the vector $\overrightarrow{OX} = \mathbf{x}$. The vector $\mathbf{x}$ is described with respect to the vector basis $\{\mathbf{a}_1, \mathbf{a}_2\}$ of $\mathbf{V}^2$ by the coefficients x_1, x_2. The coordinate system $(O, \mathbf{a}_1, \mathbf{a}_2)$ of the point space E^2 consists of the point O of E^2 and the vector basis $\{\mathbf{a}_1, \mathbf{a}_2\}$ of $\mathbf{V}^2$.

An instruction assigning uniquely to each point X of the point space E^n an 'image' point $\tilde{X}$, whereby all distances are left invariant, is called an *isometry*, an *isometric mapping* or a *motion* M of E^n. Motions are invertible, *i.e.*, for a given motion $\mathsf{M} : X \rightarrow \tilde{X}$, the inverse motion $\mathsf{M}^{-1} : \tilde{X} \rightarrow X$ exists and is unique.

Referred to a coordinate system $(O, \mathbf{a}_1, \ldots, \mathbf{a}_n)$, any motion $X \rightarrow \tilde{X}$ may be described in the form

$$\begin{array}{lcccccc} \tilde{x}_1 & = & W_{11}x_1 & + \ldots + & W_{1n}x_n & + & w_1 \\ \vdots & = & \vdots & & \vdots & & \vdots \\ \tilde{x}_n & = & W_{n1}x_1 & + \ldots + & W_{nn}x_n & + & w_n. \end{array}$$

In matrix formulation, this is expressed as

$$\begin{pmatrix} \tilde{x}_1 \\ \vdots \\ \tilde{x}_n \end{pmatrix} = \begin{pmatrix} W_{11} & \ldots & W_{1n} \\ \vdots & & \vdots \\ W_{n1} & \ldots & W_{nn} \end{pmatrix} \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix} + \begin{pmatrix} w_1 \\ \vdots \\ w_n \end{pmatrix}$$

or, in abbreviated form, as $\tilde{\boldsymbol{x}} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{w}$, where $\tilde{\boldsymbol{x}}$, $\boldsymbol{x}$ and $\boldsymbol{w}$ are all $(n \times 1)$ columns and $\boldsymbol{W}$ is an $(n \times n)$ square matrix. One often writes this in even more condensed form as $\tilde{\boldsymbol{x}} = (\boldsymbol{W}, \boldsymbol{w})\boldsymbol{x}$, or $\tilde{\boldsymbol{x}} = (\boldsymbol{W}|\boldsymbol{w})\boldsymbol{x}$; here, $(\boldsymbol{W}|\boldsymbol{w})$ is called the *Seitz symbol*.

A motion consists of a *rotation part* or *linear part* and a *translation part*. If the motion is represented by $(\boldsymbol{W}, \boldsymbol{w})$, the matrix $\boldsymbol{W}$ describes the rotation part of the motion and is called the *matrix part* of $(\boldsymbol{W}, \boldsymbol{w})$. The column $\boldsymbol{w}$ describes the translation part of the motion and is called the *vector part* or *column part* of $(\boldsymbol{W}, \boldsymbol{w})$. For a given motion, the matrix $\boldsymbol{W}$ depends only on the choice of the basis vectors, whereas the column $\boldsymbol{w}$ in general depends on the choice of the basis vectors *and* of the origin O; *cf.* Section 8.3.1.

It is possible to combine the $(n \times 1)$ column and the $(n \times n)$ matrix representing a motion into an $(n+1) \times (n+1)$ square matrix which is called the *augmented matrix*. The system of equations $\tilde{\boldsymbol{x}} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{w}$ may then be expressed in the following form:

$$\left(\begin{array}{c} \tilde{x}_1 \\ \vdots \\ \tilde{x}_n \\ \hline 1 \end{array}\right) = \left(\begin{array}{c|c} & w_1 \\ \boldsymbol{W} & \vdots \\ & w_n \\ \hline 0 \ldots 0 & 1 \end{array}\right) \left(\begin{array}{c} x_1 \\ \vdots \\ x_n \\ \hline 1 \end{array}\right)$$

or, in abbreviated form, by $\tilde{\mathbb{x}} = \mathbb{W}\mathbb{x}$. The augmentation is done in two steps. First, the $(n \times 1)$ column $\boldsymbol{w}$ is attached to the $(n \times n)$ matrix and then the matrix is made square by attaching the $[1 \times (n+1)]$ row $(0 \ldots 0\ 1)$. Similarly, the $(n \times 1)$ columns $\boldsymbol{x}$ and $\tilde{\boldsymbol{x}}$

* For this volume, the following conventions for the writing of vectors and matrices have been adopted:

(i) point coordinates and vector coefficients are written as $(n \times 1)$ column matrices;

(ii) the vectors of the vector basis are written as a $(1 \times n)$ row matrix;

(iii) *all* running indices are written as subscripts.

It should be mentioned that other conventions are also found in the literature, *e.g.* interchange of row and column matrices and simultaneous use of subscripts and superscripts for running indices.

have to be augmented to $[(n+1)\times 1]$ columns $\mathbb{x}$ and $\tilde{\mathbb{x}}$. The motion is now described by the one matrix $\mathbb{W}$ instead of the pair $(\boldsymbol{W}, \boldsymbol{w})$.

If the motion M is described by $\mathbb{W}$, the 'inverse motion' M^{-1} is described by $\mathbb{W}^{-1}$, where $(\boldsymbol{W},\boldsymbol{w})^{-1} = (\boldsymbol{W}^{-1}, -\boldsymbol{W}^{-1}\boldsymbol{w})$. Successive application of two motions, W_1 and W_2, results in another motion W_3:

$$\tilde{X} = \mathsf{W}_1 X \text{ and } \tilde{\tilde{X}} = \mathsf{W}_2\tilde{X} = \mathsf{W}_2\mathsf{W}_1 X = \mathsf{W}_3 X.$$

with $\mathsf{W}_3 = \mathsf{W}_2\mathsf{W}_1$.

This can be described in matrix notation as follows

$$\tilde{\boldsymbol{x}} = \boldsymbol{W}_1\boldsymbol{x} + \boldsymbol{w}_1$$

and

$$\tilde{\tilde{\boldsymbol{x}}} = \boldsymbol{W}_2\tilde{\boldsymbol{x}} + \boldsymbol{w}_2 = \boldsymbol{W}_2\boldsymbol{W}_1\boldsymbol{x} + \boldsymbol{W}_2\boldsymbol{w}_1 + \boldsymbol{w}_2 = \boldsymbol{W}_3\boldsymbol{x} + \boldsymbol{w}_3,$$

with $(\boldsymbol{W}_3, \boldsymbol{w}_3) = (\boldsymbol{W}_2\boldsymbol{W}_1, \boldsymbol{W}_2\boldsymbol{w}_1 + \boldsymbol{w}_2)$ or

$$\tilde{\mathbb{x}} = \mathbb{W}_1\mathbb{x} \text{ and } \tilde{\tilde{\mathbb{x}}} = \mathbb{W}_2\tilde{\mathbb{x}} = \mathbb{W}_2\mathbb{W}_1\mathbb{x} = \mathbb{W}_3\mathbb{x}$$

with $\mathbb{W}_3 = \mathbb{W}_2\mathbb{W}_1$.

It is a special advantage of the augmented matrices that successive application of motions is described by the product of the corresponding augmented matrices.

A point X is called a *fixed point* of the mapping M if it is invariant under the mapping, *i.e.* $\tilde{X} = X$.

In an n-dimensional Euclidean space E^n, three types of motions can be distinguished:

(1) *Translation.* In this case, $\boldsymbol{W} = \boldsymbol{I}$, where $\boldsymbol{I}$ is the unit matrix; the vector $\mathbf{w} = w_1\mathbf{a}_1 + \ldots + w_n\mathbf{a}_n$ is called the *translation vector.*

(2) *Motions with at least one fixed point.* In E^1, E^2 and E^3, such motions are called proper motions or *rotations* if $\det(\boldsymbol{W}) = +1$ and improper motions if $\det(\boldsymbol{W}) = -1$. Improper motions are called *inversions* if $\boldsymbol{W} = -\boldsymbol{I}$; *reflections* if $\boldsymbol{W}^2 = \boldsymbol{I}$ and $\boldsymbol{W} \neq -\boldsymbol{I}$; and *rotoinversions* in all other cases. The inversion is a rotation for spaces of even dimension, but an (improper) motion of its own kind in spaces of odd dimension. The origin is among the fixed points if $\boldsymbol{w} = \boldsymbol{o}$, where $\boldsymbol{o}$ is the $(n\times 1)$ column consisting entirely of zeros.

(3) *Fixed-point-free motions which are not translations.* In E^3, they are called *screw rotations* if $\det(\boldsymbol{W}) = +1$ and *glide reflections* if $\det(\boldsymbol{W}) = -1$. In E^2, only glide reflections occur. No such motions occur in E^1.

In Fig. 8.1.2.2, the relations between the different types of motions in E^3 are illustrated. The diagram contains all kinds of motions except the identity mapping I which leaves the whole space invariant and which is described by $\mathbb{W} = \mathbb{I}$. Thus, it is simultaneously a special rotation (with rotation angle 0) and a special translation (with translation vector $\mathbf{o}$).

So far, motions M in point space E^n have been considered. Motions give rise to mappings of the corresponding vector space $\mathbf{V}^n$ onto itself. If M maps the points P_1 and Q_1 of E^n onto P_2 and Q_2, the vector $\overrightarrow{P_1Q_1}$ is mapped onto the vector $\overrightarrow{P_2Q_2}$. If the motion in E^n is described by $\tilde{\boldsymbol{x}} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{w}$, the vectors $\mathbf{v}$ of $\mathbf{V}^n$ are mapped according to $\tilde{\mathbf{v}} = \boldsymbol{W}\mathbf{v}$. In other words, of the linear and translation parts of the motion of E^n, only the linear part remains in the corresponding mapping of $\mathbf{V}^n$ (*linear mapping*). This difference between the mappings in the two spaces is particularly obvious for translations. For a translation T with translation vector $\mathbf{t} \neq \mathbf{o}$, no fixed point exists in E^n, *i.e.* no point of E^n is mapped onto itself by T. In $\mathbf{V}^n$, however, any vector $\mathbf{v}$ is mapped onto itself since the corresponding linear mapping is the identity mapping.

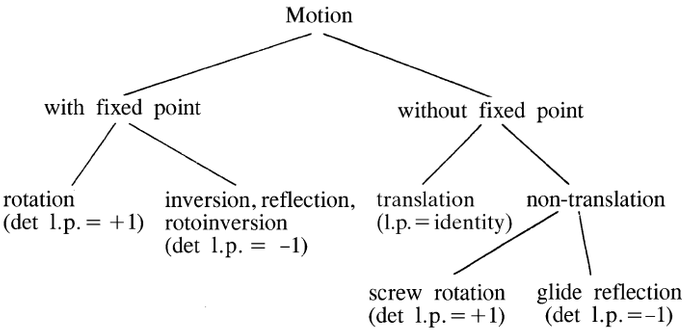

Fig. 8.1.2.2. Relations between the different kinds of motions in E^3; det l.p. = determinant of the linear part. The identity mapping does not fit into this scheme properly and hence has been omitted.

8.1.3. Symmetry operations and symmetry groups

Definition: A *symmetry operation* of a given object in point space E^n is a motion of E^n which maps this object (point, set of points, crystal pattern *etc.*) onto itself.

Remark: Any motion may be a symmetry operation, because for any motion one can construct an object which is mapped onto itself by this motion.

For the set of *all* symmetry operations of a given object, the following relations hold:

(*a*) successive application of two symmetry operations of an object results in a third symmetry operation of that object;

(*b*) the inverse of a symmetry operation is also a symmetry operation;

(*c*) there exists an 'identity operation' I which leaves each point of the space fixed: $X \rightarrow X$. This operation I is described (in any coordinate system) by $(\boldsymbol{W},\boldsymbol{w}) = (\boldsymbol{I},\boldsymbol{o})$ or by $\mathbb{W} = \mathbb{I}$ and it is a symmetry operation of any object.

(*d*) The 'associative law' $(\mathsf{W}_3\mathsf{W}_2)\mathsf{W}_1 = \mathsf{W}_3(\mathsf{W}_2\mathsf{W}_1)$ is valid.

One can show, however, that in general the 'commutative law' $\mathsf{W}_2\mathsf{W}_1 = \mathsf{W}_1\mathsf{W}_2$ is not obeyed for symmetry operations.

The properties (*a*) to (*d*) are the group axioms. Thus, the set of all symmetry operations of an object forms a group, *the symmetry group of the object* or its *symmetry.* The mathematical theorems of *group theory*, therefore, may be applied to the symmetries of objects.

So far, only rather general objects have been considered. Crystallographers, however, are particularly interested in the symmetries of crystals. In order to introduce the concept of crystallographic symmetry operations, crystal structures, crystal patterns and lattices have to be taken into consideration. This will be done in the following section.

8.1.4. Crystal patterns, vector lattices and point lattices

Crystals are finite real objects in physical space which may be idealized by infinite three-dimensional periodic 'crystal structures' in point space. Three-dimensional periodicity means that there are translations among the symmetry operations of the object with the translation vectors spanning a three-dimensional space. Extending this concept of crystal structure to more general periodic objects and to n-dimensional space, one obtains the following definition:

Definition: An object in n-dimensional point space E^n is called an n-dimensional *crystallographic pattern* or, for short, *crystal pattern* if among its symmetry operations

(i) there are n translations, the translation vectors $\mathbf{t}_1, \ldots, \mathbf{t}_n$ of which are linearly independent,