International Tables for Crystallography (2006). Vol. D, Section 3.2.3.2, pp. 381–385.

the image of exactly one element of A, then the mapping φ becomes a *one-to-one correspondence between* A *and* B, $\varphi : \mathsf{A} \leftrightarrow \mathsf{B}$. In this case, A and B are of the same order.

One often encounters a situation in which one assigns to each ordered pair $(\mathbf{S}, \mathbf{M})$ an element $\mathbf{N}$, where all three elements $\mathbf{S}, \mathbf{M}, \mathbf{N}$ are elements from the same set A, symbolically $\varphi : (\mathbf{S}, \mathbf{M}) \mapsto \mathbf{N}$; $\mathbf{S}, \mathbf{M}, \mathbf{N} \in \mathsf{A}$ or $\varphi : \mathsf{A} \times \mathsf{A} \to \mathsf{A}$. Such a mapping is called a *binary operation* or a *composition law* on the set A. A sum of two numbers $a + b = c$ or a product of two numbers $a \cdot b = c$, where a, b, c belong to the set of all real numbers, are elementary examples of binary operations.

3.2.3.1.4. *Equivalence relation on a set, partition of a set*

The notion of the ordered pair allows one to introduce another useful concept, namely the relation on a set. An example will illustrate this notion. Let $\mathbb{Z}$ be a set of integers, $\mathbb{Z} = \{\ldots, -2, -1, 0, 1, 2, \ldots\}$. For each ordered pair (m, n), $m, n \in \mathbb{Z}$, one can decide whether m is smaller than n, $m < n$, or not. All pairs (m, n) that fulfil the condition $m < n$ form a subset R of all possible ordered pairs $\mathbb{Z} \times \mathbb{Z}$. In other words, the relation $m < n$ defines a subset R of the set $\mathbb{Z} \times \mathbb{Z}$, $\mathsf{R} \subset \mathbb{Z} \times \mathbb{Z}$. Similarly, the relation $|m| = |n|$ ($|n|$ denotes absolute value of n) defines another subset of $\mathbb{Z} \times \mathbb{Z}$.

To indicate that an element $\mathbf{S}$ is related to $\mathbf{M}$ by $\overset{\mathsf{R}}{\sim}$, where $\mathbf{S}, \mathbf{M} \in \mathsf{A}$, one writes $\mathbf{S} \overset{\mathsf{R}}{\sim} \mathbf{M}$, where the relation R defines a subset R of all ordered pairs $\mathsf{A} \times \mathsf{A}$, $\mathsf{R} \subset \mathsf{A} \times \mathsf{A}$ (the same letter R is used for the subset and for the relation on A). The opposite also holds: Each subset R of $\mathsf{A} \times \mathsf{A}$ defines a certain relation $\overset{\mathsf{R}}{\sim}$ on A.

A relation $\overset{\mathsf{R}}{\sim}$ is called an *equivalence relation on the set* A if it satisfies three conditions:

$$\mathbf{S} \overset{\mathsf{R}}{\sim} \mathbf{S} \text{ for all } \mathbf{S} \in \mathsf{A} \ (\textit{reflexivity}), \quad (3.2.3.3)$$

$$\text{if } \mathbf{S}, \mathbf{M} \in \mathsf{A} \text{ and } \mathbf{S} \overset{\mathsf{R}}{\sim} \mathbf{M}, \text{ then } \mathbf{M} \overset{\mathsf{R}}{\sim} \mathbf{S} \ (\textit{symmetry}), \quad (3.2.3.4)$$

$$\text{if } \mathbf{S}, \mathbf{M}, \mathbf{N} \in \mathsf{A}, \ \mathbf{S} \overset{\mathsf{R}}{\sim} \mathbf{M} \text{ and } \mathbf{M} \overset{\mathsf{R}}{\sim} \mathbf{N}, \text{ then } \mathbf{S} \overset{\mathsf{R}}{\sim} \mathbf{N} \ (\textit{transitivity}). \quad (3.2.3.5)$$

Thus, for example, it is easy to corroborate that the relation $|m| = |n|$ on the set of integers $\mathbb{Z}$ fulfils all three conditions (3.2.3.3) to (3.2.3.5) and is, therefore, an equivalence relation on the set $\mathbb{Z}$. On the other hand, the relation $m < n$ is not an equivalence relation on $\mathbb{Z}$ since it fulfils neither the reflexivity (3.2.3.3) nor the symmetry condition (3.2.3.4).

Let $\overset{\mathsf{R}}{\sim}$ be an equivalence relation on A and $\mathbf{S} \in \mathsf{A}$; all elements $\mathbf{M} \in \mathsf{A}$ such that $\mathbf{M} \overset{\mathsf{R}}{\sim} \mathbf{S}$ constitute a subset of A denoted $[\mathbf{S}]_{\mathsf{R}}$ and called the *equivalence class of* $\mathbf{S}$ *with respect to* $\overset{\mathsf{R}}{\sim}$ (or the R-*equivalence class of* $\mathbf{S}$). The element $\mathbf{S}$ is called the *representative* of the class $[\mathbf{S}]_{\mathsf{R}}$. Any other member of the class can be chosen as its representative. Any two elements of the equivalence class $[\mathbf{S}]_{\mathsf{R}}$ are R-*equivalent elements of* A.

From the definition of the equivalence class, it follows that any two elements $\mathbf{M}, \mathbf{N} \in \mathsf{A}$ are either R-equivalent elements of A, $\mathbf{M} \overset{\mathsf{R}}{\sim} \mathbf{N}$, and thus belong to the same class, $[\mathbf{M}]_{\mathsf{R}} = [\mathbf{N}]_{\mathsf{R}}$, or are not R-equivalent, and thus belong to two different classes that are disjoint, $[\mathbf{M}]_{\mathsf{R}} \cap [\mathbf{N}]_{\mathsf{R}} = \emptyset$. In this way, the equivalence relation $\overset{\mathsf{R}}{\sim}$ divides the set A into disjoint subsets (equivalence classes), the union of which is equal to the set itself. Such a decomposition is called a *partition of the set* A *associated with the equivalence relation* $\overset{\mathsf{R}}{\sim}$. For a finite set A this decomposition can be expressed as a union of equivalence classes,

$$\mathsf{A} = [\mathbf{S}]_{\mathsf{R}} \cup [\mathbf{M}]_{\mathsf{R}} \cup \ldots \cup [\mathbf{Q}]_{\mathsf{R}}, \quad (3.2.3.6)$$

where $\mathbf{S}, \mathbf{M}, \ldots, \mathbf{Q}$ are representatives of the equivalence classes.

Generally, any decomposition of a set into a system of disjoint non-empty subsets such that every element of the set is a member of just one subset is called a *partition of the set*. To any partition of a set A there corresponds an equivalence relation $\overset{\mathsf{R}}{\sim}$ such that the R-equivalence classes of A form that partition. This equivalence relation defines two elements as equivalent if and only if they belong to the same subset.

The term 'equivalent' is often used when it is clear from the context what the relevant equivalence relation is. Similarly, the term 'class' is used instead of 'equivalence class'. Sometimes equivalence classes have names that do not explicitly indicate that they are equivalence classes. For example, in group theory, conjugate subgroups, left, right and double cosets form equivalence classes (see Section 3.2.3.2). Often instead of the expression 'partition of a set A' an equivalent expression 'classification of the elements of a set A' is used. The most important equivalence classes in the symmetry analysis of domain structures are called orbits and will be discussed in Section 3.2.3.3.

More details on set theory can be found in Kuratowski & Mostowski (1968), Lipschutz (1981), and Opechowski (1986).

3.2.3.2. *Groups and subgroups*

3.2.3.2.1. *Groups*

Operations (isometries) that act on a body without changing its form and internal state combine in the same way as do elements of a group. Group theory is, therefore, the main mathematical tool for examining transformation properties – symmetry properties in particular – of crystalline objects. The basic concept of group theory is that of a group.

Definition 3.2.3.2. A *group* G is a set that satisfies four postulates:

(1) To each ordered pair (g_i, g_j) of two elements of G, there corresponds a unique element g_k of G, *i.e.* a binary operation (composition law) is defined on the set G. Usually, one writes the ordered pair simply as a 'product' g_ig_j and the composition law as an equation,

$$g_ig_j = g_k, \quad g_i, g_j, g_k \in G. \quad (3.2.3.7)$$

This condition is referred to as *closure of G under multiplication.*

(2) The *multiplication is associative*, *i.e.* for any three elements g_i, g_j, g_k of G it holds that if $g_ig_j = g_l$ and $g_jg_k = g_m$ then $g_lg_k = g_ig_m$. This condition is usually written as one equation,

$$(g_ig_j)g_k = g_i(g_jg_k), \quad (3.2.3.8)$$

which expresses the requirement that the product of any three elements of G is the same, no matter which two of the three one multiplies first, as long as the order in which they stand is not changed. From postulate (2) it follows that the product of any finite sequence of group elements is determined uniquely if the order in which the elements are placed is preserved.

(3) The set G contains an *identity* or *unit element* e such that

$$eg = ge = g \text{ for any element } g \in G. \quad (3.2.3.9)$$

(4) For any element $g \in G$ there exists an *inverse element* g^{-1} such that

$$gg^{-1} = g^{-1}g = e. \quad (3.2.3.10)$$

The number of elements of a group G is called the *order of the group*. If the order of the group is finite, it is denoted by $|G|$.

The multiplication of group elements is, in general, not commutative, *i.e.* $g_ig_j \neq g_jg_i$ may hold for some $g_i, g_j \in G$. If the multiplication is commutative, *i.e.* if $g_ig_j = g_jg_i$ for all $g_i, g_j \in G$, then the group G is called a *commutative* or *Abelian group*. All groups of orders 1 to 5 are Abelian. In Abelian groups, an *additive notation* is sometimes used instead of the *multiplicative notation*, *i.e.* if g_i and g_k are elements of an Abelian group G then one writes $g_i + g_k$ instead of $g_i g_k$. Additive notation is usually used in groups of translations.

The *nth power* g^n of an element $g \in G$, where n is a positive integer, is defined recursively in the following manner:

(i) $g^0 = e$, $g^1 = g$, where e is a unit element of G;
(ii) $g^{n+1} = g^n g$;
(iii) $g^{-n} = (g^n)^{-1}$.

If G is written additively, one writes ng instead of g^n and speaks of a *multiple of g*.

If m and n are integers and g is an element of G then the following *laws of exponents* hold:

$$g^m g^n = g^{m+n} = g^n g^m, \tag{3.2.3.11}$$
$$(g^m)^n = g^{mn} = (g^n)^m. \tag{3.2.3.12}$$

A set of elements $\{g_1, g_2, \ldots\}$ of a group G is called a *set of generators of G* if any element of the group G can be written as a product of powers of these generators. In general, a group may have several sets of generators.

The *order of an element g* is the smallest positive integer m such that $g^m = e$. An element g and the inverse element g^{-1} have the same order. The order m of any element g of a finite group G is a factor of the order $|G|$.

Two groups G and G' with elements $g_1, g_2, \ldots, g_i, \ldots$ and $g'_1, g'_2, \ldots, g'_i, \ldots$, respectively, are *isomorphic* if there is an one-to-one correspondence φ between G and G',

$$\varphi : g_i \leftrightarrow g'_i \text{ for each } \; g_i \in G, \tag{3.2.3.13}$$

such that

$$\text{whenever } \varphi : g_i \leftrightarrow g'_i \text{ and } \varphi : g_j \leftrightarrow g'_j, \text{ then } \varphi : g_i g_j \leftrightarrow g'_i g'_j. \tag{3.2.3.14}$$

In other words, the *isomorphism of two groups G and G′* is a one-to-one mapping of G onto G' [(3.2.3.13)] which preserves the products of the elements of the two groups [(3.2.3.14)]. Two isomorphic groups G and G' are denoted as $G \cong G'$.

Isomorphism is an equivalence relation that divides the set of all groups into classes of isomorphic groups. Between two groups G and G' there may exist several isomorphisms.

Groups that appear in Chapters 3.3 and 3.4 are mostly *crystallographic groups* [for their definition and properties see Bradley & Cracknell (1972), Hahn & Wondratschek (1994), *IT* A (2002), *IT* A1 (2003), Janssen (1973), Opechowski (1986), and Vainshtein (1994)]. Elements of these groups are distance-preserving transformations (mappings) called *isometries*, *Euclidean transformations*, *motions* or *crystallographic operations*. Whenever we encounter crystallographic groups we shall use the term 'crystallographic operation' or just 'operation' or 'isometry' instead of 'element'.

In what follows, the group G may be a crystallographic point group or a crystallographic space group. Since we shall be mainly concerned with a continuum approach, we shall have in mind point groups. When we consider space groups, we shall mention this explicitly and, if possible, use calligraphic letters, *e.g.* $\mathcal{G}$, $\mathcal{F}$ *etc.* for space groups.

Crystallographic operations of crystallographic point groups and products of these operations can be found by means of the multiplication calculator in the software *GI★KoBo*-1 under the menu item *Group Elements* (see the manual for *GI★KoBo*-1).

3.2.3.2.2. *Subgroups*

Definition 3.2.3.3. Let G be a group. A subset F of G is a *subgroup of G* if it forms a group under the product rule of G, *i.e.* if it fulfils the group postulates (1) to (4).

For finite groups these requirements can be replaced by a single condition [see *e.g.* Opechowski (1986)]: The product of any two elements f_i, f_j of F belongs to F,

$$f_i f_j = f_k, \quad f_k \in F \text{ for any } f_i, f_j \in F. \tag{3.2.3.15}$$

The groups G and F are denoted the *high-symmetry group* and the *low-symmetry group*, respectively. The pair '*group G – subgroup F*' is called the *symmetry descent* $G \supset F$, *dissymmetrization* $G \supset F$ or *symmetry reduction* $G \supset F$. A symmetry descent is a basic specification of a phase transition and corresponding domain structure (see Chapters 3.1 and 3.4).

Each group G always has at least two subgroups: the group G itself (sometimes called the *improper subgroup*) and the *trivial subgroup* consisting of the unit element only. The symbol $F \subseteq G$ signifies that F is a subgroup of G including the improper subgroup G, whereas $F \subset G$ means that F is a *proper subgroup* of G which differs from G. By this definition, the trivial subgroup is a proper subgroup. This definition of a proper subgroup [used *e.g.* in Volume A of the present series (*IT* A, 2002) and by Opechowski (1986)] is convenient for our purposes, although often by the term 'proper subgroup' one understands a subgroup different from G and from the trivial subgroup.

A proper subgroup F of G is a *maximal subgroup of G* if it is not a proper subgroup of some other proper subgroup H, *i.e.* if there exists no group H such that $F \subset H \subset G$. A group can have more than one maximal subgroup.

A group P for which G is subgroup is called a *supergroup of G*, $G \subseteq P$. If G is a proper subgroup of Q, $G \subset Q$, then Q is a *proper supergroup of G*. If G is a maximal subgroup of P, then P is called a *minimal supergroup of G*.

Let a group L be a proper supergroup of a group F, $F \subset L$, and simultaneously a proper subgroup of a group G, $L \subset G$. Then the sequence of subgroups

$$F \subset L \subset G \tag{3.2.3.16}$$

will be called a *group–subgroup chain* and the group L an *intermediate group* of the chain (3.2.3.16).

Subgroups of crystallographic point groups are listed in Table 3.4.2.7 and are displayed in Figs. 3.1.3.1 and 3.1.3.2 (see also the software *GI★KoBo*-1, menu item *Subgroups*).

3.2.3.2.3. *Left and right cosets*

If F_1 is a proper subgroup of G and g_i is a fixed element of G, then the set of all products $g_i f$, where f runs over all elements of the subgroup F_1, is denoted $g_i F_1$ and is called the *left coset of* F_1 *in G*,

$$g_i F_1 = \{g_i f \,|\, \forall f \in F_1\}, \quad g_i \in G, \quad F_1 \subset G, \tag{3.2.3.17}$$

where the sign $\forall$ means 'for all'. Similarly, one defines a *right coset of* F_1 *in G*:

$$F_1 g_i = \{f g_i \,|\, \forall f \in F_1\}, \quad g_i \in G, \quad F_1 \subset G. \tag{3.2.3.18}$$

[Some authors, *e.g.* Hall (1959), call the set $g_i F_1$ a right coset of F_1 in G and the set $F_1 g_i$ a left coset of F_1 in G.] Since in the application of cosets in the symmetry analysis of domain structures left cosets are used almost exclusively, all statements that follow are formulated for left cosets. Each statement about left cosets has a complementary statement about right cosets which can in most cases be obtained by replacing 'left' with 'right'.

The element g_i which appears explicitly in the symbol $g_i F_1$ of the left coset of F_1 is called a *representative of the left coset* $g_i F_1$. Any element of a left coset can be chosen as its representative.

Left coset criterion: Two elements g_i and g_j belong to the same left coset, $g_i F_1 = g_j F_1$, if and only if $g_i^{-1} g_j$ belongs to the subgroup F_1, $g_i^{-1} g_j \in F_1$.

The property of 'belong to the same left coset' is an equivalence relation, therefore two left cosets of the same subgroup are either identical or have no elements in common.

Proposition 3.2.3.4. The union of all distinct left cosets of F_1 in G constitutes a partition of G and is called the *decomposition of G into the left cosets of* F_1. If the set of left cosets of F_1 in G is finite, then the decomposition of G into the left cosets of F_1 can be expressed as

$$G = g_1F_1 \cup g_2F_1 \cup \ldots \cup g_nF_1 = \bigcup_{i=1}^{n} g_iF_1, \qquad (3.2.3.19)$$

where the symbol $\cup$ is the set-theoretical union (see Section 3.2.3.1). For the representative g_1 of the first left coset the unit element e is usually chosen, $g_1 = e$. Then the first left coset is identical with the subgroup F_1. The number of elements in each left coset of the decomposition is equal to the order of the group F_1.

The set of left-coset representatives $\{g_1, g_2, \ldots g_n\}$ is sometimes called a *left transversal to* F_1 *in* G.

The number n of distinct left cosets is called the *index of the subgroup* F_1 *in the group* G and is denoted by the symbol $[G:F_1]$. If the groups G and F_1 are of finite order then

$$n = [G:F_1] = |G| : |F_1|, \qquad (3.2.3.20)$$

where $|G|$ and $|F_1|$ are the orders of G and F_1, respectively. From this equation follows:

Lagrange's theorem: the order of a finite group is a multiple of the order of each of its subgroups. Alternatively, the index of a subgroup and the order of a finite subgroup are divisors of the group order.

We note that an infinite subgroup of an infinite group can have a finite index. Important examples are subgroups of translational groups of crystallographic space groups and subgroups of space groups (see Example [oC] 3.2.3.32 in Section 3.2.3.3.5).

The decompositions of crystallographic point groups into left and right cosets are available in the software *GI★KoBo*-1, under *Subgroups\View\Twinning Group*.

Proposition 3.2.3.5. Let L_1 be an intermediate group $F_1 \subset L_1 \subset G$. The group G can be decomposed into left cosets of L_1,

$$G = h_1L_1 \cup h_2L_1 \cup \ldots \cup h_mL_1 = \bigcup_{j=1}^{m} h_jL_1, \qquad (3.2.3.21)$$

where

$$m = [G:L_1] = |G| : |L_1|, \qquad (3.2.3.22)$$

and the group L_1 into left cosets of F_1,

$$L_1 = p_1F_1 \cup p_2F_1 \cup \ldots \cup p_dF_1 = \bigcup_{k=1}^{d} p_kF_1, \qquad (3.2.3.23)$$

where

$$d = [L_1:F_1] = |L_1| : |F_1|. \qquad (3.2.3.24)$$

Then the decomposition of G into left cosets of F_1 can be written in the form

$$G = \bigcup_{j=1}^{m}\bigcup_{k=1}^{d} h_jp_kF_1 \qquad (3.2.3.25)$$

and the index n of F_1 in G can be expressed as a product of indices m and d,

$$n = [G:F_1] = [G:L_1][L_1:F_1] = md. \qquad (3.2.3.26)$$

Decompositions (3.2.3.19) and (3.2.3.21) of a group into left cosets enable one to divide a set of objects into classes of symmetrically equivalent objects (see Section 3.2.3.3.4). The concept of domain states is based on this result (see Section 3.4.2).

3.2.3.2.4. *Conjugate subgroups*

Two subgroups F_i and F_k are *conjugate subgroups* if there exists an element g of G such that

$$gF_ig^{-1} = F_k, \quad g \in G. \qquad (3.2.3.27)$$

More explicitly, one says that the subgroup F_k is *conjugate by g* (or *conjugate under G*) *to the subgroup* F_i. Conjugate subgroups are isomorphic.

The property of 'being conjugate' is an equivalence relation. The set of all subgroups of a group G can therefore be partitioned into disjoint classes of conjugate subgroups. Conjugate subgroups of crystallographic point groups are given in Table 3.4.2.7 and in the software *GI★KoBo*-1, under *Subgroups\View\Twinning Group.*

3.2.3.2.5. *Normalizers*

The collection of all elements g that fulfil the relation

$$gF_ig^{-1} = F_i, \quad g \in G, \qquad (3.2.3.28)$$

constitutes a group denoted by $N_G(F_i)$ and is called the *normalizer of* F_i *in G. The normalizer* $N_G(F_i)$ *is a subgroup of G and a supergroup of* F_i,

$$F_i \subseteq N_G(F_i) \subseteq G. \qquad (3.2.3.29)$$

The normalizer $N_G(F_i)$ determines the subgroups conjugate to F_i under G (see Example 3.2.3.10). The number m of subgroups conjugate to a subgroup F_i under G equals the index of $N_G(F_i)$ in G:

$$m = [G:N_G(F_i)] = |G| : |N_G(F_i)|, \qquad (3.2.3.30)$$

where the last equation holds for finite G and F_i.

Normalizers of the subgroups of crystallographic point groups are available in Table 3.4.2.7 and in the software *GI★KoBo*-1 under *Subgroups\View\Twinning Group*.

3.2.3.2.6. *Normal subgroups*

Among subgroups of a group, a special role is played by normal subgroups. A subgroup H of G is a *normal* (*invariant*, *self-conjugate*) *subgroup* of G if and only if it fulfils any of the following conditions:

(1) The subgroup H of G has no conjugate subgroups under G. (No subscript is therefore needed in the symbol of a normal subgroup H.)

(2) The normalizer $N_G(H)$ of H equals the group G,

$$N_G(H) = G. \qquad (3.2.3.31)$$

(3) Every element g of G commutes with H, or, equivalently, each left coset gH equals the right coset Hg:

$$gH = Hg \text{ for every } g \in G. \qquad (3.2.3.32)$$

For a normal subgroup H of a group G a special symbol $\triangleleft$ is often used instead of $\subset$, $H \triangleleft G$.

3.2.3.2.7. *Halving subgroups and dichromatic (black-and-white) groups*

Any subgroup H of a group G of index 2, called a *halving subgroup*, is a normal subgroup. The decomposition of G into left cosets of H consists of two left cosets,

$$G = H \cup gH. \qquad (3.2.3.33)$$

Sometimes it is convenient to distinguish elements of the coset gH from elements of the halving subgroup H. This can be achieved by attaching a sign (usually written as a superscript) to all elements of the coset. We shall use for this purpose the sign $\spadesuit$. To aid understanding, we shall also mark for a while the elements of the group H with another sign, $\heartsuit$. The multiplication law for these 'decorated elements' can be written in the following form:

$$g_1^{\heartsuit}g_2^{\heartsuit} = g_3^{\heartsuit}, \quad g_4^{\heartsuit}g_5^{\spadesuit} = g_6^{\spadesuit}, \quad g_7^{\spadesuit}g_8^{\heartsuit} = g_9^{\spadesuit}, \quad g_{10}^{\spadesuit}g_{11}^{\spadesuit} = g_{12}^{\heartsuit}. \qquad (3.2.3.34)$$

Now we replace the label $\heartsuit$ by a dummy 'no mark' sign (*i.e.* we remove $\heartsuit$), but we still keep in mind the multiplication rules (3.2.3.34). Then the decomposition (3.2.3.33) becomes

$$G = H \cup g^{\spadesuit}H, \qquad (3.2.3.33a)$$

since the coset $g^{\spadesuit}H$ assembles all marked elements and H consists of all bare elements of the group G.

The sign $\spadesuit$ can carry useful additional information, *e.g.* the application of labelled operations $g^{\spadesuit}$ is connected with some changes or new effects, whereas the application of a bare operation brings about no such changes or effects.

The label $\spadesuit$ can be replaced by various signs which can have different meanings. Thus in Chapter 3.3 a prime $'$ signifies a nontrivial twinning operation, in Chapter 1.5 it is associated with time inversion in magnetic structures, and in black-and-white patterns or structures a prime denotes an operation which exchanges black and white 'colours' (the qualifier 'black-and-white' concerns group operations, but not the black-and-white pattern itself). In Chapter 3.4, a star * denotes a transposing operation which exchanges two domain states, while underlining signifies an operation exchanging two sides of an interface and underlined operations with a star signify twinning operations of a domain twin. Various interpretations of the label attached to the symbol of an operation have given rise to several designations of groups with partition (3.2.3.34): *black-and-white*, *dichromatic*, *magnetic*, *anti-symmetry*, *Shubnikov* or *Heech–Shubnikov* and other *groups*. For more details see Opechowski (1986).

3.2.3.2.8. *Double cosets*

Let F_1 and H_1 be two proper subgroups of the group G. The set of all distinct products hg_jf, where g_j is a fixed element of the group G and f and h run over all elements of the subgroups F_1 and H_1, respectively, is called a *double coset of F_1 and H_1 in G*. The symbol of this double coset is $H_1g_jF_1$,

$$F_1g_jH_1 = \{fg_jh \,|\, \forall f \in F_1, \forall h \in H_1\},$$
$$g_j \in G,\ F_1 \subset G,\ H_1 \subset G, \qquad (3.2.3.35)$$

where the sign $\forall$ means 'for all'.

In the symmetry analysis of domain structures, only double cosets with $H_1 = F_1$ are used. We shall, therefore, formulate subsequent definitions and statements only for this special type of double coset.

The fixed element g_j is called the *representative of the double coset $F_1g_jF_1$*. Any element of a double coset can be chosen as its representative.

Two double cosets are either identical or disjoint.

Proposition 3.2.3.6. The union of all distinct double cosets constitutes a partition of G and is called the *decomposition of the group G into double cosets of* F_1, since $F_1F_1 = F_1$. If the set of double cosets of F_1 in G is finite, then the decomposition of G into the double cosets of F_1 can be written as

$$G = F_1g_1F_1 \cup F_1g_2F_1 \cup \ldots \cup F_1g_qF_1. \qquad (3.2.3.36)$$

For the representative g_1 of the first double coset $F_1g_jF_1$ the unit element e is usually chosen, $g_1 = e$. Then the first double coset is identical with the subgroup F_1.

A double coset $F_1g_jF_1$ consists of left cosets of the form fg_jF_1, where $f \in F_1$. The number r of left cosets of F_1 in the double coset $F_1g_jF_1$ is (Hall, 1959)

$$r = [F_1 : F_{1j}], \qquad (3.2.3.37)$$

where

$$F_{1j} = F_1 \cap g_jF_1g_j^{-1}. \qquad (3.2.3.38)$$

The following definitions and statements are used in Chapter 3.4 for the double cosets $F_1g_jF_1$ [for derivations and more details, see Janovec (1972)].

The inverse $(F_1g_jF_1)^{-1}$ of a double coset $F_1g_jF_1$ is a double coset $F_1g_j^{-1}F_1$, which is either identical or disjoint with the double coset $F_1g_jF_1$. The double coset that is its own inverse is called an *invertible* (*self-inverse*, *ambivalent*) *double coset*. The double coset that is disjoint with its inverse is called a *non-invertible* (*polar*) *double coset* and the double cosets $F_1g_jF_1$ and $(F_1g_jF_1)^{-1} = F_1g_j^{-1}F_1$ are called *complementary polar double cosets*.

The inverse left coset $(g_jF_1)^{-1}$ contains representatives of all left cosets of the double coset $F_1g_j^{-1}F_1$. If a left coset g_jF_1 belongs to an invertible double coset, then $(g_jF_1)^{-1}$ contains representatives of left cosets constituting the double coset $F_1g_jF_1$. If a left coset g_jF_1 belongs to a non-invertible double coset, then $(g_jF_1)^{-1}$ contains representatives of left cosets constituting the complementary double coset $(F_1g_jF_1)^{-1}$.

A double coset consisting of only one left coset,

$$F_1g_jF_1 = g_jF_1, \qquad (3.2.3.39)$$

is called a simple *double coset*. A double coset $F_1g_jF_1$ is *simple* if and only if the inverse $(g_jF_1)^{-1}$ of the left coset g_jF_1 is again a left coset. For an invertible simple double coset $g_jF_1 = (g_jF_1)^{-1}$.

The union of all simple double cosets $F_1g_jF_1 = g_jF_1$ in the double coset decomposition of G (3.2.3.36) constitutes the normalizer $N_G(F_1)$ (Speiser, 1927).

A double coset that comprises more than one left coset will be called a *multiple double coset*. Four types of double cosets FgF are displayed in Table 3.2.3.1. The double coset decompositions of all crystallographic point groups are available in the software *GI*★*KoBo*-1 under *Subgroups\View\Twinning Group*.

Double cosets and the decomposition (3.2.3.36) of a group in double cosets are mathematical tools for partitioning a set of pairs of objects into equivalent classes (see Section 3.2.3.3.6). Such a division enables one to find possible twin laws and different types of domain walls that can appear in a domain structure resulting from a phase transition with a given symmetry descent (see Chapters 3.3 and 3.4).

More detailed introductions to group theory can be found in Budden (1972), Janssen (1973), Ledermann (1973), Rosen (1995), Shubnikov & Koptsik (1974), Vainshtein (1994) and Vainshtein *et*

Table 3.2.3.1. *Four types of double cosets*

	$FgF = gF$	$FgF \neq gF$
$FgF = (FgF)^{-1}$	Invertible simple	Invertible multiple
$FgF \cap (FgF)^{-1} = \emptyset$	Non-invertible simple	Non-invertible multiple

al. (1995). More advanced books on group theory are, for example, Bradley & Cracknell (1972), Hall (1959), Lang (1965), Opechowski (1986), Robinson (1982) and Speiser (1927). Parts of group theory relevant to phase transitions and tensor properties are treated in the manual of the software *GI⋆KoBo*-1. Representations of the crystallographic groups are presented in Chapter 1.2 of this volume and in the software *GI⋆KoBo*-1 (see the manual).

3.2.3.3. *Action of a group on a set*

3.2.3.3.1. *Group action*

A direct application of the set and group theory to our studies would hardly justify their presentation in the last two sections. However, an appropriate combination of these theories, called group action, forms a very useful tool for examining crystalline materials and domain structures in particular. In this section, the main concepts (action of a group on a set [a], orbits [o], stabilizers [s]) are explained and their application is illustrated with examples from crystallography, where the group G is either a crystallographic point group or space group (denoted $\mathcal{G}$, if necessary), and the set is the three-dimensional point space $E(3)$ [P], a crystal [C], a property tensor [T] and a subgroup of G [S]. Letters in square brackets in front of the sequential number of examples and definitions should aid navigation in the text.

Example [aP] 3.2.3.7. Crystals are objects in a three-dimensional space called point space. Points of this space form an infinite set which we denote $E(3)$. If one chooses a point O as the origin, then to each point $X \in E(3)$ one can assign the position vector $OX = \mathbf{r}$ of a vector space $V(3)$ [see, for example, *IT* A (2002), Part 8]. There is a one-to-one correspondence between points of the point space and corresponding position vectors of the vector space,

$$X \leftrightarrow OX = \mathbf{r}. \qquad (3.2.3.40)$$

If one further selects three non-coplanar basic vectors $\mathbf{e_1}, \mathbf{e_2}, \mathbf{e_3}$, then the position vector $\mathbf{r}$ can be written as

$$\mathbf{r} = x_1\mathbf{e}_1 + x_2\mathbf{e}_2 + x_3\mathbf{e}_3, \qquad (3.2.3.41)$$

where x_1, x_2, x_3 are coordinates of the point X.

Let G be a point group. An operation (isometry) $g \in G$ transforms (moves) the point X to a point X' with the position vector

$$\mathbf{r}' = x_1'\mathbf{e}_1 + x_2'\mathbf{e}_2 + x_3'\mathbf{e}_3. \qquad (3.2.3.42)$$

Coordinates of this image point are related to coordinates of the initial point by a linear relation,

$$x_i' = \sum_{j=1}^{3} D(g)_{ij}x_j, \quad i = 1, 2, 3, \qquad (3.2.3.43)$$

where $D(g)_{ij}$ are components of a 3×3 matrix representing the operation g.

The described motion of the point X under the operation g can be formally expressed as a simple relation

$$gX = X', \quad g \in G, \quad X, X' \in E(3), \qquad (3.2.3.44)$$

the exact meaning of which can be formulated in terms introduced in Section 3.2.3.1 as a mapping φ that assigns to an ordered pair (g, X) a point X' of the set $E(3)$,

$$\varphi : (g, X) \longmapsto X', \quad g \in G \text{ and } X, X' \in \mathsf{A}. \qquad (3.2.3.45)$$

The mapping φ – *i.e.* a prescription for how to determine from g and X the resulting point X' – is defined by (3.2.3.40) to (3.2.3.43). The relation (3.2.3.44) should be considered as only a shorthand version of the explicit relation (3.2.3.45).

The action of a group on a set generalizes the described procedure to any group and any set. In this section, we shall use the term 'object' for an element of a set and the term 'operation' for an element of a group.

Definition [a] 3.2.3.8. Let G be a group, A a set of objects $\mathbf{S}_i, \mathbf{S}_j, \mathbf{S}_k, \ldots$ and $\varphi : G \times \mathsf{A} \rightarrow \mathsf{A}$ a mapping that assigns to an ordered pair $(g, \mathbf{S}_i)$, where $g \in G$, S_i and S_i are objects of the set A:

$$\varphi : (g, \mathbf{S}_i) \longmapsto \mathbf{S}_k, \quad g \in G, \quad \mathbf{S}_i, \mathbf{S}_k \in \mathsf{A}. \qquad (3.2.3.46)$$

The ordered pair $(g, \mathbf{S}_i)$ can often be written simply as a product $g\mathbf{S}_i$ and the mapping as an equation. Then the relation (3.2.3.46) can be expressed in a simpler form:

$$g\mathbf{S}_i = \mathbf{S}_k, \quad g \in G, \ \mathbf{S}_i, \mathbf{S}_k \in \mathsf{A}. \qquad (3.2.3.47)$$

If the mapping (3.2.3.46), expressed in this condensed way, fulfils two additional conditions,

$$e\mathbf{S}_i = \mathbf{S}_i \text{ for any } \mathbf{S}_i \in \mathsf{A}, \qquad (3.2.3.48)$$

where e is the identity operation (unit element) of G, and

$$h(g\mathbf{S}_i) = (hg)\mathbf{S}_i \text{ for any } h, g \in G \text{ and any } \mathbf{S}_i \in \mathsf{A}, \qquad (3.2.3.49)$$

then the mapping φ is called an *action* (or *operation*) *of a group G on a set* A, or just a *group action*.

We must note that the replacement of the explicit mapping (3.2.3.46) by a contracted version (3.2.3.47) is not always possible (see Example [aS] 3.2.3.11).

The condition (3.2.3.49) requires that the first action $g\mathbf{S}_i = \mathbf{S}_k$ followed by the second action $h\mathbf{S}_k = \mathbf{S}_m$ gives the same result as if one first calculates the product $hg = p$ and then applies it to $\mathbf{S}_i$, $p\mathbf{S}_i = \mathbf{S}_m$.

When a group G, a set A, and a mapping φ fulfil the requirements (3.2.3.47) to (3.2.3.49), one says that *G acts* or *operates on* A and the set A is called a *G-set*.

Example [aC] 3.2.3.9. We shall examine the action of an isometry g on an ideal infinite crystal in the three-dimensional space. Let us choose four points (atoms) of the crystal that define three non-coplanar vectors $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ (*e.g.* basic lattice translations). These vectors will specify the *orientation of the crystal in space*. Let g be a point-group operation. This isometry g transforms (moves) points of the crystal to new positions and changes the orientation of the crystal to a new orientation specified by vectors $\mathbf{a}_1', \mathbf{a}_2', \mathbf{a}_3'$,

$$\mathbf{a}_i' = \sum_{j=3}^{3} D(g)_{ji}\mathbf{a}_j, \quad i = 1, 2, 3, \qquad (3.2.3.50)$$

where $D(g)_{ji}$ are coefficients of a 3×3 matrix representing the operation g. For non-trivial operations g, the resulting vectors $\mathbf{a}_1', \mathbf{a}_2', \mathbf{a}_3'$ always differ from the initial ones. If g is an improper rotation (rotoinversion), then these vectors have an opposite handedness to the vectors $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ of the initial orientation and, for enantiomorphous crystals, the transformed crystal is an enantiomorphous form of the crystal in the initial orientation.

We choose a *reference coordinate system* defined by the origin O and by three non-coplanar basis vectors $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$. By the *state* $\boldsymbol{S}$ *of a crystal* we shall understand, in a continuum description, the set of all its properties expressed by components of physical property (matter) tensors in the reference coordinate system or, in a microscopic description, the positions of atoms in the elementary unit cell expressed in the reference coordinate system. States defined in this way may change with temperature and external fields, and also with the orientation of the crystal in