International Tables for Crystallography (2006). Vol. D, Section 3.2.3.2.3, pp. 382–383.

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:

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

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',

$$\varphi : g_i \leftrightarrow g'_i \text{ for each } g_i \in G, \qquad (3.2.3.13)$$

such that

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

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,

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

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

$$F \subset L \subset G \qquad (3.2.3.16)$$

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*,

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

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

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

[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 $\lhd$ is often used instead of $\subset$, $H \lhd G$.

references