

3. PHASE TRANSITIONS, TWINNING AND DOMAIN STRUCTURES

one writes $g_i + g_k$ instead of $g_i g_k$. Additive notation is usually used in groups of translations.

The n th 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:

$$g^m g^n = g^{m+n} = g^n g^m, \quad (3.2.3.11)$$

$$(g^m)^n = g^{mn} = (g^n)^m. \quad (3.2.3.12)$$

A set of elements $\{g_1, g_2, \dots\}$ 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 $g_1, g_2, \dots, g_i, \dots$ and $g'_1, g'_2, \dots, g'_i, \dots$, respectively, are *isomorphic* if there is an one-to-one correspondence φ between G and G' ,

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

such that

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

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 ,

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

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

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

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* ,

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

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

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

[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 , $g_i^{-1} g_j \in F_1$.