

## 3.2. TWINNING AND DOMAIN STRUCTURES

state  $\mathbf{S}_1$  by the stabilizer  $\mathcal{I}_G(\mathbf{S}_1) = \mathcal{F}_1$ . The stabilizer of the primary order parameter  $\eta^{(1)}$  must fulfil the condition

$$I_G(\eta^{(1)}) = I_G(\mathbf{S}_1) = \mathcal{F}_1. \quad (3.2.3.57)$$

The appearance of nonzero  $\eta^{(1)}$  in the ferroic phase thus fully accounts for the symmetry descent  $\mathcal{G} \supset \mathcal{F}_1$  at the transition.

In a continuum description, a role analogous to  $\eta^{(1)}$  is played by a *principal tensor parameter*  $\mu^{(1)}$  (see Section 3.1.3). Its stabilizer  $I_G(\mu^{(1)})$  in the parent point group  $G$  equals the point group  $F_1$  of the first single domain state  $\mathbf{S}_1$ ,

$$I_G(\mu^{(1)}) = I_G(\mathbf{S}_1) = F_1. \quad (3.2.3.58)$$

This contrasts with the *secondary order parameter*  $\lambda^{(1)}$  (*secondary tensor parameter* in a continuum description). Its stabilizer

$$I_G(\lambda^{(1)}) = L_1 \quad (3.2.3.59)$$

is an intermediate group  $F_1 \subset L_1 \subset G$ , *i.e.* the appearance of  $\lambda^{(1)}$  would lead only to a partial symmetry descent  $G \supset L_1$  with  $L_1 \supset F_1$ .

*Example [sS] 3.2.3.17.* The stabilizer of a subgroup  $F_i \subset G$  from Example [aS] 3.2.3.11 is the normalizer  $N_G(F_i)$  defined in Section 3.2.3.2.5:

$$I_G(F_i) = \{g \in G | gF_i g^{-1} = F_i\} = N_G(F_i). \quad (3.2.3.60)$$

In general, a stabilizer, which is a subgroup of  $G$ , is an example of a structure which is induced by a group action on the group  $G$ . On the other hand, a group action exerts a partition of the set  $\mathbf{A}$  into equivalence classes called orbits.

## 3.2.3.3.3. Orbits

The group action allows one to specify the equivalence relation and the partition of a set into equivalence classes introduced in Section 3.2.3.1 [see (3.2.3.6)]. If  $G$  is a group and  $\mathbf{S}_i, \mathbf{S}_k$  are two objects of a  $G$ -set  $\mathbf{A}$ , then one says that the *objects*  $\mathbf{S}_i, \mathbf{S}_k$  are *G-equivalent*,  $\mathbf{S}_i \stackrel{G}{\sim} \mathbf{S}_k$ , if there exists an operation  $g \in G$  that transforms  $\mathbf{S}_i$  into  $\mathbf{S}_k$ ,

$$\mathbf{S}_k = g\mathbf{S}_i, \quad \mathbf{S}_i, \mathbf{S}_k \in \mathbf{A}, \quad g \in G. \quad (3.2.3.61)$$

In our applications, the group  $G$  is most often a crystallographic group. In this situation we shall speak about *crystallographically equivalent objects*. Exceptionally,  $G$  will be the group of all isometries  $O(3)$  (full orthogonal group in three dimensions); then we shall talk about *symmetrically equivalent objects*.

The relation  $\stackrel{G}{\sim}$  is an equivalence relation on a set  $\mathbf{A}$  and therefore divides a set  $\mathbf{A}$  into  $G$ -equivalence classes. These classes are called orbits and are defined in the following way:

*Definition [o] 3.2.3.18.* Let  $\mathbf{A}$  be a  $G$ -set and  $\mathbf{S}_i$  an object of the set  $\mathbf{A}$ . A *G orbit* of  $\mathbf{S}_i$ , denoted  $G\mathbf{S}_i$ , is a set of all objects of  $\mathbf{A}$  that are  $G$ -equivalent with  $\mathbf{S}_i$ ,

$$G\mathbf{S}_i = \{g\mathbf{S}_i | \forall g \in G\}, \quad \mathbf{S}_i \in \mathbf{A}. \quad (3.2.3.62)$$

*Important note:* The object  $\mathbf{S}_i$  of the orbit  $G\mathbf{S}_i$  is called the *representative of the orbit*  $G\mathbf{S}_i$ . If the group  $G$  is known from the context, one simply speaks of an *orbit of*  $\mathbf{S}_i$ .

Any two objects of an orbit are  $G$ -equivalent and any object of the orbit can be chosen as a representative of this orbit. Two  $G$  orbits  $G\mathbf{S}_r, G\mathbf{S}_s$  of a  $G$ -set  $\mathbf{A}$  are either identical or disjoint. The set  $\mathbf{A}$  can therefore be partitioned into disjoint orbits,

$$\mathbf{A} = G\mathbf{S}_i \cup G\mathbf{S}_k \cup \dots \cup G\mathbf{S}_q. \quad (3.2.3.63)$$

Different groups  $G$  produce different partitions of the set  $\mathbf{A}$ .

*Example [oP] 3.2.3.19.* If  $X$  is a point in three-dimensional point space and  $G$  is a crystallographic point group (see Example [aP] 3.2.3.7), then the orbit  $G(X)$  consisting of all crystallographically equivalent points is called a *point form* [see *IT A* (2002), Part 10]. If the group is a space group  $\mathcal{G}$ , then  $\mathcal{G}(X)$  is called the *crystallographic orbit of*  $X$  with respect to  $\mathcal{G}$ . In this case, the crystallographic orbit is an infinite set of points due to the infinite number of translations in the space group  $\mathcal{G}$  [see *IT A* (2002), Part 8]. In this way, the infinite set of points of the point space is divided into an infinite number of disjoint orbits.

*Example [oC] 3.2.3.20.* Let  $\mathbf{S}_1$  be a domain state from Example [aC] 3.2.3.9. The orbit  $G\mathbf{S}_1$ , where  $G$  is the parent phase symmetry, assembles all  $G$ -equivalent domain states,

$$G\mathbf{S}_1 = \{\mathbf{S}_1, \mathbf{S}_2, \dots, \mathbf{S}_n\}. \quad (3.2.3.64)$$

The existence of several equivalent states is the main characteristic feature of domain states. Domain states of the orbit  $G\mathbf{S}_1$  represent all possible variants of the low-symmetry phase with the same energy and the same chance of appearance in the domain structure. Structurally, they represent the crystal structure  $\mathbf{S}_1$  in all distinguishable orientations (and also positions in a microscopic description) related by isometries of the group  $G$ . If  $G$  contains rotoinversions and if  $\mathbf{S}_1$  is an enantiomorphic structure, then the orbit  $G\mathbf{S}_1$  also comprises the enantiomorphic form of  $\mathbf{S}_1$ .

*Example [oT] 3.2.3.21.* Let  $\mu^{(1)}$  be a principal tensor parameter of the point-group-symmetry descent  $G \supset F_1$  (see Example [sT] 3.2.3.16). The orbit  $G\mu^{(1)}$  consists of all points in the tensor space of the principal tensor parameter that are crystallographically equivalent with respect to  $G$ ,

$$G\mu^{(1)} = \{\mu^{(1)}, \mu^{(2)}, \dots, \mu^{(n)}\}. \quad (3.2.3.65)$$

*Example [oS] 3.2.3.22.* The orbit  $GF_1$  of a subgroup  $F_1$  in Example [aS] 3.2.3.11 is the set of all subgroups conjugate under  $G$  to  $F_1$ ,

$$GF_1 = \{F_1, g_2 F_1 g_2^{-1}, \dots, g_m F_1 g_m^{-1}\}. \quad (3.2.3.66)$$

From Proposition 3.2.3.13 and from Example [oS] 3.2.3.22, it follows that stabilizers of objects from one orbit  $G\mathbf{S}_i$  constitute the orbit (3.2.3.66) of all subgroups conjugate under  $G$ . One can thus associate with each orbit  $G\mathbf{S}_i$  an orbit  $GF_i$  of conjugate subgroups of  $G$ . The set of all objects with stabilizers from one orbit  $GF_i$  of conjugate subgroups is called a *stratum of*  $F_i$  *in the set*  $\mathbf{A}$  (Michel, 1980; Kerber, 1999). In crystallography, the term *Wyckoff position* is used for the stratum of points of the point space (*IT A*, 2002).

The notion of a stratum can be also applied to the classification of orbits of domain states treated in Example [oC] 3.2.3.22. Let  $G$  be the symmetry of the parent phase and  $\mathbf{A}$  the set of all states of the crystal. Orbits  $G\mathbf{S}_i$  of domain states with stabilizers from one orbit  $GF_i$  of conjugate subgroups of  $G$ ,  $F_i = I_G(\mathbf{S}_i)$ , are of the 'same type' and form a *stratum of domain states*. Domain states of different orbits belonging to the same stratum differ in the numerical values of parameters describing the states but have the same crystallographic and topological properties. All possible strata that can be formed from a given parent phase with

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symmetry  $G$  can be identified with all different orbits of subgroups of  $G$ .

In a similar manner, points of the order-parameter space and tensor-parameter space from Examples [sC] 3.2.3.16 and [oT] 3.2.3.21 can be divided into strata which are characterized by the orbits of possible stabilizers.

Next, we formulate three propositions that are essential in the symmetry analysis of domain structures presented in Section 3.4.2.

#### 3.2.3.3.4. Orbits and left cosets

*Proposition 3.2.3.23.* Let  $G$  be a finite group,  $\mathbf{A}$  a  $G$ -set and  $I_G(\mathbf{S}_1) \equiv F_1$  the stabilizer of an object  $\mathbf{S}_1$  of the set  $\mathbf{A}$ ,  $\mathbf{S}_1 \in \mathbf{A}$ . The objects of the orbit

$$G\mathbf{S}_1 = \{\mathbf{S}_1, \mathbf{S}_2, \dots, \mathbf{S}_j, \dots, \mathbf{S}_n\} \quad (3.2.3.67)$$

and the left cosets  $g_j F_1$  of the decomposition of  $G$ ,

$$G = g_1 F_1 \cup g_2 F_1 \cup \dots \cup g_j F_1 \cup \dots \cup g_n F_1 = \bigcup_{j=1}^n g_j F_1, \quad (3.2.3.68)$$

are in a one-to-one correspondence,

$$\mathbf{S}_j \leftrightarrow g_j F_1, \quad F_1 = I_G(\mathbf{S}_1), \quad j = 1, 2, \dots, n. \quad (3.2.3.69)$$

(See *e.g.* Kerber, 1991, 1999; Kopský, 1983; Lang, 1965.) The derivation of the bijection (3.2.3.69) consists of two parts:

(i) All operations of a left coset  $g_j F_1$  transform  $\mathbf{S}_1$  into the same  $\mathbf{S}_j = g_j \mathbf{S}_1$ , since  $g_j \mathbf{S}_1 = g_j (F_1 \mathbf{S}_1) = (g_j F_1) \mathbf{S}_1$ , where we use the relation

$$\begin{aligned} F_1 \mathbf{S}_1 &= \{f_1, f_2, \dots, f_q\} \mathbf{S}_1 \\ &= \{f_1 \mathbf{S}_1, f_2 \mathbf{S}_1, \dots, f_q \mathbf{S}_1\} \\ &= \{\mathbf{S}_1, \mathbf{S}_1, \dots, \mathbf{S}_1\} = \{\mathbf{S}_1\} = \mathbf{S}_1, \end{aligned} \quad (3.2.3.70)$$

which in the second line contains a generalization of the group action and in the third line reflects Definition 3.2.3.1 of a set as a collection of distinguishable objects,  $\{\mathbf{S}_1, \mathbf{S}_1, \dots, \mathbf{S}_1\} = \mathbf{S}_1 \cup \mathbf{S}_1 \dots \cup \mathbf{S}_1 = \mathbf{S}_1$ .

(ii) Any  $g_r \in G$  that transforms  $\mathbf{S}_1$  into  $\mathbf{S}_j = g_j \mathbf{S}_1$  belongs to the left coset  $g_j F_1$ , since from  $g_j \mathbf{S}_1 = g_r \mathbf{S}_1$  it follows that  $g_r^{-1} g_j \mathbf{S}_1 = \mathbf{S}_1$ , *i.e.*  $g_r^{-1} g_j \in F_1$ , which, according to the left coset criterion, holds if and only if  $g_r$  and  $g_j$  belong to the same left coset  $g_j F_1$ .

We note that the orbit  $G\mathbf{S}_1$  depends on the stabilizer  $I_G(\mathbf{S}_1) = F_1$  of the object  $\mathbf{S}_1$  and not on the ‘eigensymmetry’ of  $\mathbf{S}_1$ .

From Proposition 3.2.3.23 follow two corollaries:

*Corollary 3.2.3.24.* The order  $n$  of the orbit  $G\mathbf{S}_1$  equals the index of the stabilizer  $I_G(\mathbf{S}_1) = F_1$  in  $G$ ,

$$n = [G : I_G(\mathbf{S}_1)] = [G : F_1] = |G| : |F_1|, \quad (3.2.3.71)$$

where the last part of the equation applies to point groups only.

*Corollary 3.2.3.25.* All objects of the orbit  $G\mathbf{S}_1$  can be generated by successive application of representatives of all left cosets  $g_j F_1$  in the decomposition of  $G$  [see (3.2.3.68)] to the object  $\mathbf{S}_1$ ,  $\mathbf{S}_j = g_j \mathbf{S}_1$ ,  $j = 1, 2, \dots, n$ . The orbit  $G\mathbf{S}_1$  can therefore be expressed explicitly as

$$G\mathbf{S}_1 = \{\mathbf{S}_1, g_2 \mathbf{S}_1, \dots, g_j \mathbf{S}_1, \dots, g_n \mathbf{S}_1\}, \quad (3.2.3.72)$$

where the operations  $g_1 = e, g_2, \dots, g_j, \dots, g_n$  (left transversal to  $F_1$  in  $G$ ) are the representatives of left cosets in the decomposition (3.2.3.68).

*Example [oP] 3.2.3.26.* The number of equivalent points of the point form  $GX$  ( $G$  orbit of the point  $X$ ) is called a *multiplicity*  $m_G(X)$  of this point,

$$m_G(X) = |G| : |I_G(X)|. \quad (3.2.3.73)$$

The multiplicity of a point of general position equals the order  $|G|$  of the group  $G$ , since in this case  $I_G(X) = e$ , a trivial group. Then points of the orbit  $GX$  and the operations of  $G$  are in a one-to-one correspondence. The multiplicity of a point of special position is smaller than the order  $|G|$ ,  $m_G(X) < |G|$ , and the operations of  $G$  and the points of the orbit  $GX$  are in a many-to-one correspondence. Points of a stratum have the same multiplicity; one can, therefore, talk about the multiplicity of the Wyckoff position [see *IT A* (2002)]. If  $G$  is a space group, the point orbit has to be confined to the volume of the primitive unit cell (Wondratschek, 1995).

*Example [oC] 3.2.3.27.* Corollaries 3.2.3.24 and 3.2.3.25 applied to domain states represent the basic relations of domain-structure analysis. According to (3.2.3.71), the index  $n$  of the stabilizer  $I_G(\mathbf{S}_1)$  in the parent group  $G$  gives the number of domain states in the orbit  $G\mathbf{S}_1$  and the relations (3.2.3.72) and (3.2.3.68) give a recipe for constructing domain states of this orbit.

*Example [oT] 3.2.3.28.* If  $\mu^{(1)}$  is a principal tensor parameter associated with the symmetry descent  $G \supset F_1$ , then there is a one-to-one correspondence between the elements of the orbit of single domain states  $G\mathbf{S}_1 = \{\mathbf{S}_1, \mathbf{S}_2, \dots, \mathbf{S}_j, \dots, \mathbf{S}_n\}$  and the elements of the orbit of the principal order parameter (points)  $G\mu^{(1)} = \{\mu^{(1)}, \mu^{(2)}, \dots, \mu^{(j)}, \dots, \mu^{(n)}\}$  (see Example [oT] 3.2.3.21),

$$\mathbf{S}_j \leftrightarrow g_j F_1 \leftrightarrow \mu^{(j)}, \quad j = 1, 2, \dots, n. \quad (3.2.3.74)$$

Therefore, single domain states of the orbit  $G\mathbf{S}_1$  can be represented by the principal tensor parameter of the orbit  $G\mu^{(1)}$ .

*Example [oS] 3.2.3.29.* Consider a subgroup  $F_1$  of a group  $G$ . Since the stabilizer of  $F_1$  in  $G$  is the normalizer  $N_G(F_1)$  (see Example [sS] 3.2.3.17), the number  $m$  of conjugate subgroups is, according to (3.2.3.71),

$$m = [G : N_G(F_1)] = |G| : |N_G(F_1)|, \quad (3.2.3.75)$$

where the last part of the equation applies to point groups only. The orbit of conjugate subgroups is

$$GF_1 = \{F_1, h_2 F_1 h_2^{-1}, \dots, h_j F_1 h_j^{-1}, \dots, h_m F_1 h_m^{-1}\}, \quad j = 1, 2, \dots, m, \quad (3.2.3.76)$$

where the operations  $h_1 = e, h_2, \dots, h_j, \dots, h_m$  are the representatives of left cosets in the decomposition

$$G = N_G(F_1) \cup h_2 N_G(F_1) \cup \dots \cup h_j N_G(F_1) \cup \dots \cup h_m N_G(F_1). \quad (3.2.3.77)$$

*3.2.3.3.5. Intermediate subgroups and partitions of an orbit into suborbits*

*Proposition 3.2.3.30.* Let  $G\mathbf{S}_1$  be a  $G$  orbit from Proposition 3.2.3.23 and  $L_1$  an intermediate group,

$$F_1 \subset L_1 \subset G. \quad (3.2.3.78)$$

A successive decomposition of  $G$  into left cosets of  $L_1$  and  $L_1$  into left cosets of  $F_1$  [see (3.2.3.25)] introduces a two-indices rela-