

## 3. PHASE TRANSITIONS, TWINNING AND DOMAIN STRUCTURES

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

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

$$j = 1, 2, \dots, m,$$

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-

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belling of the objects of a  $G$  orbit defined by the one-to-one correspondence

$$h_j p_k F_1 \leftrightarrow \mathbf{S}_{jk}, \quad j = 1, 2, \dots, m, \quad k = 1, 2, \dots, d, \quad (3.2.3.79)$$

where  $\{h_1, h_2, \dots, h_m\}$  are the representatives of the decompositions of  $G$  into left cosets of  $L_1$ ,

$$G = h_1 L_1 \cup h_2 L_1 \cup \dots \cup h_j L_1 \cup \dots \cup h_m L_1, \quad m = [G : L_1], \quad (3.2.3.80)$$

and  $\{p_1, p_2, \dots, p_d\}$  are the representatives of the decompositions of  $L_1$  into left cosets of  $F_1$ ,

$$L_1 = p_1 F_1 \cup p_2 F_1 \cup \dots \cup p_k F_1 \cup \dots \cup p_d F_1, \quad d = [L_1 : F_1]. \quad (3.2.3.81)$$

The index  $n$  of  $F_1$  in  $G$  can be expressed as a product of indices  $m$  and  $d$  [see (3.2.3.26)],

$$n = [G : F_1] = [G : L_1][L_1 : F_1] = md. \quad (3.2.3.82)$$

If  $G$  is a finite group, then the index  $n$  can be expressed in terms of orders of groups  $G$ ,  $F_1$  and  $L_1$ :

$$n = |G| : |F_1| = (|G| : |L_1|)(|L_1| : |F_1|) = md. \quad (3.2.3.83)$$

When one chooses  $\mathbf{S}_1 = \mathbf{S}_{11}$ , then the members of the orbit  $G\mathbf{S}_{11}$  can be arranged into an  $m \times d$  array,

$$\begin{array}{cccccc} \mathbf{S}_{11} & \mathbf{S}_{12} & \dots & \mathbf{S}_{1k} & \dots & \mathbf{S}_{1d} \\ \mathbf{S}_{21} & \mathbf{S}_{22} & \dots & \mathbf{S}_{2k} & \dots & \mathbf{S}_{2d} \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\ \mathbf{S}_{j1} & \mathbf{S}_{j2} & \dots & \mathbf{S}_{jk} & \dots & \mathbf{S}_{jd} \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\ \mathbf{S}_{m1} & \mathbf{S}_{m2} & \dots & \mathbf{S}_{mk} & \dots & \mathbf{S}_{md} \end{array} \quad (3.2.3.84)$$

The set of objects of the  $j$ th row of this array forms an  $L_j$  orbit with the representative  $\mathbf{S}_{j1}$ ,

$$\begin{aligned} \{\mathbf{S}_{j1}, \mathbf{S}_{j2}, \dots, \mathbf{S}_{jk}, \dots, \mathbf{S}_{jd}\} \\ = \{h_j p_1 \mathbf{S}_{11}, h_j p_2 \mathbf{S}_{11}, \dots, h_j p_k \mathbf{S}_{11}, \dots, h_j p_d \mathbf{S}_{11}\} \\ = L_j \mathbf{S}_{j1}, \end{aligned} \quad (3.2.3.85)$$

where

$$L_j = h_j L_1 h_j^{-1}, \quad \mathbf{S}_{j1} = h_j \mathbf{S}_{11}, \quad j = 1, 2, \dots, m. \quad (3.2.3.86)$$

The intermediate group  $L_1$  thus induces a *splitting of the orbit*  $G\mathbf{S}_{11}$  into  $m$  suborbits  $L_j \mathbf{S}_{j1}$ ,  $j = 1, 2, \dots, m$ :

$$G\mathbf{S}_{11} = L_1 \mathbf{S}_{11} \cup L_2 \mathbf{S}_{21} \cup \dots \cup L_j \mathbf{S}_{j1} \cup \dots \cup L_m \mathbf{S}_{m1}, \quad m = [G : L_1]. \quad (3.2.3.87)$$

Aizu (1972) denotes this partitioning *factorization of species*.

The relation (3.2.3.79) is just the application of the correspondence (3.2.3.69) of Proposition 3.2.3.23 on the successive decomposition (3.2.3.25). Derivation of the second part of Proposition 3.2.3.30 can be sketched in the following way:

$$\begin{aligned} \{\mathbf{S}_{j1}, \mathbf{S}_{j2}, \dots, \mathbf{S}_{jd}\} &= h_j \{p_1 \mathbf{S}_{11}, p_2 \mathbf{S}_{11}, \dots, p_d \mathbf{S}_{11}\} \\ &= h_j \{p_1, p_2, \dots, p_d\} F_1 \mathbf{S}_{11} \\ &= h_j L_1 \mathbf{S}_{11} = h_j L_1 h_j^{-1} \mathbf{S}_{j1} = L_j \mathbf{S}_{j1}, \\ j &= 1, 2, \dots, m, \end{aligned} \quad (3.2.3.88)$$

where the relation (3.2.3.70) is used.

We note that the described partitioning of an orbit into suborbits depends on the choice of representative of the first suborbit  $\mathbf{S}_{11}$  and that the number of conjugate subgroups  $L_j$  may be equal to or smaller than the number  $m$  of suborbits (see Example [oS] 3.2.3.34).

Each intermediate group  $L_1$  in Proposition 3.2.3.30 can usually be associated with a certain attribute, e.g. a secondary order parameter, which specifies the suborbits.

*Example [oP] 3.2.3.31.* Let  $G$  be a point group and  $X_1$  a point of general position ( $I_G(X_1) = e$ ) in the point space. A symmetry descent to a subgroup  $L_1 \subset G$  is accompanied by a splitting of the orbit  $GX_1$  of  $|G|$  equivalent points into  $m = |G| : |L_1|$  suborbits each consisting of  $|L_1|$  equivalent points. The first suborbit is  $L_1 X_1$ , the others are  $L_j X_j$ ,  $L_j = h_j L_1 h_j^{-1}$ ,  $X_j = h_j X_1$ ,  $j = 1, 2, \dots, m$ , where  $h_j$  are representatives of left cosets of  $L_1$  in the decomposition of  $G$  [see (3.2.3.80)].

Splitting of orbits of points of general position is a special case in which  $I_L(X_1) = I_G(X_1)$ . Splitting of orbits of points of special position is more complicated if  $I_L(X_1) \subset I_G(X_1)$  (see Wondratschek, 1995).

*Example [oC] 3.2.3.32.* Let us consider a phase transition accompanied by a lowering of space-group symmetry from a parent space group  $\mathcal{G}$  with translation subgroup  $\mathbf{T}$  and point group  $G$  to a low-symmetry space group  $\mathcal{F}$  with translation subgroup  $\mathbf{U}$  and point group  $F$ . There exists a unique intermediate group  $\mathcal{M}$ , called the *group of Hermann*, which has translation subgroup  $\mathbf{T}$  and point group  $M = F$  (see e.g. Hahn & Wondratschek, 1994; Wadhawan, 2000; Wondratschek & Aroyo, 2001).

The decomposition of  $\mathcal{G}$  into left cosets of  $\mathcal{M}$ , corresponding to (3.2.3.80), is in a one-to-one correspondence with the decomposition of  $G$  into left cosets of  $F$ , since  $\mathcal{G}$  and  $\mathcal{M}$  have the same translation subgroup  $\mathbf{T}$  and  $\mathcal{M}$  and  $\mathcal{F}$  have the same point group. Therefore, the index  $n \equiv [\mathcal{G} : \mathcal{M}] = [G : F] = |G| : |F|$ .

Since  $\mathcal{M}$  and  $\mathcal{F}$  have the same point group  $F$ , the decomposition of  $\mathcal{M}$  into left cosets of  $\mathcal{F}$ , corresponding to (3.2.3.81), is in a one-to-one correspondence with the decomposition of  $\mathbf{T}$  into left cosets of  $\mathbf{U}$ ,

$$\mathbf{T} = \mathbf{t}_1 \mathbf{U} + \mathbf{t}_2 \mathbf{U} + \dots + \mathbf{t}_d \mathbf{U}. \quad (3.2.3.89)$$

Representatives  $\mathbf{t}_1, \mathbf{t}_2, \dots, \mathbf{t}_d$  are translations. The corresponding vectors lead from the origin of a 'superlattice' primitive unit cell of the low-symmetry phase to lattice points of  $\mathbf{T}$  located within or on the side faces of this 'superlattice' primitive unit cell (Van Tendeloo & Amelinckx, 1974). The number  $d_i$  of these vectors is equal to the ratio  $v_{\mathcal{F}} : v_{\mathcal{G}} = Z_{\mathcal{F}} : Z_{\mathcal{G}}$ , where  $v_{\mathcal{F}}$  and  $v_{\mathcal{G}}$  are the volumes of the *primitive* unit cell of the low-symmetry phase and the parent phase, respectively, and  $Z_{\mathcal{F}}$  and  $Z_{\mathcal{G}}$  are the number of chemical formula units in the *primitive* unit cell of the low-symmetry phase and the parent phase, respectively.

There is another useful formula for expressing  $d_i = [\mathbf{T} : \mathbf{U}]$ . The primitive basis vectors  $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$  of  $\mathbf{U}$  are related to the primitive basis vectors  $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$  of  $\mathbf{T}$  by a linear relation,

$$\mathbf{b}_i = \sum_{j=1}^3 \mathbf{a}_j m_{ij}, \quad i = 1, 2, 3, \quad (3.2.3.90)$$

where  $m_{ij}$  are integers. The volumes of primitive unit cells are  $v_{\mathcal{G}} = \mathbf{a}_1(\mathbf{a}_2 \times \mathbf{a}_3)$  and  $v_{\mathcal{F}} = \mathbf{b}_1(\mathbf{b}_2 \times \mathbf{b}_3)$ . Using (3.2.3.90), one gets  $v_{\mathcal{F}} = \det(m_{ij})v_{\mathcal{G}}$ , where  $\det(m_{ij})$  is the determinant of the  $(3 \times 3)$  matrix of the coefficients  $m_{ij}$ . Hence the index  $d_i = (v_{\mathcal{F}} : v_{\mathcal{G}}) = \det(m_{ij})$ .

Thus we get for the index  $N$  of  $\mathcal{F}$  in  $\mathcal{G}$

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$$\begin{aligned} N &= [G : \mathcal{F}] = [G : F][\mathbf{T} : \mathbf{U}] \\ &= (|G| : |F|)(v_{\mathcal{F}} : v_G) = (|G| : |F|)(Z_{\mathcal{F}} : Z_G) \\ &= (|G| : |F|)\det(m_{ij}) = nd_i. \end{aligned} \quad (3.2.3.91)$$

Each suborbit, represented by a row in the array (3.2.3.84), contains all basic (microscopic) domain states that are related by pure translations. These domain states exhibit the same tensor properties, *i.e.* they belong to the same ferroic domain state.

*Example [sT] 3.2.3.33.* Let us consider a phase transition with a symmetry descent  $G \supset F_1$  with an orbit  $G\mathbf{S}_{11}$  of domain states. Let  $L_1$  be an intermediate group,  $F_1 \subset L_1 \subset G$ , and  $\lambda^{(1)}$  the principal order parameter associated with the symmetry descent  $G \supset L_1$  [cf. (3.2.3.58)],  $I_G(\lambda^{(1)}) = L_1$ . Since  $L_1$  is an intermediate group, the quantity  $\lambda^{(1)}$  represents a secondary order parameter of the symmetry descent  $G \supset F_1$ . The  $G$  orbit of  $\lambda^{(1)}$  is

$$G\lambda^{(1)} = \{\lambda^{(1)}, \lambda^{(2)}, \dots, \lambda^{(m)}\}, \quad m = [G : L_1]. \quad (3.2.3.92)$$

As in Example [oT] 3.2.3.28, there is a bijection between left cosets of the decomposition of  $G$  into left cosets of  $L_1$  [see (3.2.3.80)] and the  $G$  orbit of secondary order parameters (3.2.3.92). One can, therefore, associate with the suborbit  $L_j\mathbf{S}_{j1}$  the value  $\lambda^{(j)}$  of the secondary order parameter  $\lambda$ ,

$$L_j\mathbf{S}_{j1} \leftrightarrow \lambda^{(j)}, \quad j = 1, 2, \dots, m. \quad (3.2.3.93)$$

A suborbit  $L_j\mathbf{S}_{j1}$  is thus comprised of objects of the orbit  $G\mathbf{S}_{11}$  with the same value of the secondary order parameter  $\lambda^{(j)}$ .

*Example [oS] 3.2.3.34.* Let us choose for the intermediate group  $L_1$  the normalizer  $N_G(F_1)$ . Then the suborbits equal

$$\begin{aligned} N_G(F_1)\mathbf{S}_{j1} &= \{h_j\mathbf{S}_{11}, h_j p_2\mathbf{S}_{11}, \dots, h_j p_d\mathbf{S}_{11}\}, \\ j &= 1, 2, \dots, m = [G : N_G(F_1)], \end{aligned} \quad (3.2.3.94)$$

where  $p_1 = e, p_2, \dots, p_d$  are representatives of left cosets  $p_k F_1$  in the decomposition of  $N_G(F_1)$ ,

$$N_G(F_1) = p_1 F_1 \cup p_2 F_1 \cup \dots \cup p_d F_1, \quad d = [N_G(F_1) : F_1], \quad (3.2.3.95)$$

and  $h_j$  are representatives of the decomposition (3.2.3.77). The suborbit  $F_j\mathbf{S}_{j1}$  consists of all objects with the same stabilizer  $F_j$ ,

$$\begin{aligned} I_G(\mathbf{S}_{j1}) &= I_G(\mathbf{S}_{j2}) = \dots = I_G(\mathbf{S}_{jd}) = F_j, \\ j &= 1, 2, \dots, m = [G : N_G(F_1)]. \end{aligned} \quad (3.2.3.96)$$

Propositions 3.2.3.23 and 3.2.3.30 are examples of structures that a group action induces from a group  $G$  on a  $G$ -set. Another important example is a permutation representation of the group  $G$  which associates operations of  $G$  with permutations of the objects of the orbit  $G\mathbf{S}_i$  [see *e.g.* Kerber (1991, 1999); for application of the permutation representation in domain-structure analysis and domain engineering, see *e.g.* Fuksa & Janovec (1995, 2002)].

#### 3.2.3.3.6. Orbits of ordered pairs and double cosets

An ordered pair  $(\mathbf{S}_i, \mathbf{S}_k)$  is formed by two objects  $\mathbf{S}_i, \mathbf{S}_k$  from the orbit  $G\mathbf{S}_1$ . Let  $\mathbf{P}$  denote the set of all ordered pairs that can be formed from the objects of the orbit  $G\mathbf{S}_1$ . The group action  $\varphi$  of group  $G$  on the set  $\mathbf{P}$  is defined by the following relation:

$$\begin{aligned} \varphi : g(\mathbf{S}_i, \mathbf{S}_k) &= (g\mathbf{S}_i, g\mathbf{S}_k) = (\mathbf{S}_r, \mathbf{S}_s), \\ g \in G, \quad (\mathbf{S}_i, \mathbf{S}_k), (\mathbf{S}_r, \mathbf{S}_s) &\in \mathbf{P}. \end{aligned} \quad (3.2.3.97)$$

The requirements (3.2.3.47) to (3.2.3.49) are fulfilled, mapping (3.2.3.97) defines an action of group  $G$  on the set  $\mathbf{P}$ .

The group action (3.2.3.97) introduces the  $G$ -equivalence of ordered pairs: Two ordered pairs  $(\mathbf{S}_i, \mathbf{S}_k)$  and  $(\mathbf{S}_r, \mathbf{S}_s)$  are crystallographically equivalent (with respect to the group  $G$ ),  $(\mathbf{S}_i, \mathbf{S}_k) \stackrel{G}{\sim} (\mathbf{S}_r, \mathbf{S}_s)$ , if there exists an operation  $g \in G$  that transforms  $(\mathbf{S}_i, \mathbf{S}_k)$  into  $(\mathbf{S}_r, \mathbf{S}_s)$ ,

$$g \in G (g\mathbf{S}_i, g\mathbf{S}_k) = (\mathbf{S}_r, \mathbf{S}_s), \quad (\mathbf{S}_i, \mathbf{S}_k), (\mathbf{S}_r, \mathbf{S}_s) \in \mathbf{P}. \quad (3.2.3.98)$$

An orbit of ordered pairs  $G(\mathbf{S}_i, \mathbf{S}_k)$  comprises all ordered pairs crystallographically equivalent with  $(\mathbf{S}_i, \mathbf{S}_k)$ . One can choose as a representative of the orbit  $G(\mathbf{S}_i, \mathbf{S}_k)$  an ordered pair  $(\mathbf{S}_1, \mathbf{S}_j)$  with the first member  $\mathbf{S}_1$  since there is always an operation  $g_{i1} \in G$  such that  $g_{i1}\mathbf{S}_i = \mathbf{S}_1$ . The orbit  $F_1(\mathbf{S}_1, \mathbf{S}_j)$  assembles all ordered pairs with the first member  $\mathbf{S}_1$ . This orbit can be expressed as

$$\begin{aligned} F_1(\mathbf{S}_1, \mathbf{S}_j) &= (F_1\mathbf{S}_1, F_1\mathbf{S}_j) = (\mathbf{S}_1, F_1(g_j\mathbf{S}_1)) \\ &= (\mathbf{S}_1, (F_1g_j)(F_1\mathbf{S}_1)) = (\mathbf{S}_1, (F_1g_jF_1)\mathbf{S}_1), \end{aligned} \quad (3.2.3.99)$$

where the identity  $F_1\mathbf{S}_1 = \mathbf{S}_1$  [see relation (3.2.3.70)] has been used.

Thus the double coset  $F_1g_jF_1$  contains all operations from  $G$  that produce all ordered pairs with the first member  $\mathbf{S}_1$  that are  $G$ -equivalent with  $(\mathbf{S}_1, \mathbf{S}_j = g_j\mathbf{S}_1)$ . If one chooses  $g_r \in G$  that is not contained in the double coset  $F_1g_jF_1$ , then the ordered pair  $(\mathbf{S}_1, \mathbf{S}_r = g_r\mathbf{S}_1)$  must belong to another orbit  $G(\mathbf{S}_1, \mathbf{S}_r) \neq G(\mathbf{S}_1, \mathbf{S}_j)$ . Hence to distinct double cosets there correspond distinct classes of ordered pairs with the first member  $\mathbf{S}_1$ , *i.e.* distinct orbits of ordered pairs. Since the group  $G$  can be decomposed into disjoint double cosets [see (3.2.3.36)], one gets

*Proposition 3.2.3.35.* Let  $G$  be a group and  $\mathbf{P}$  a set of all ordered pairs that can be formed from the objects of the orbit  $G\mathbf{S}_1$ . There is a one-to-one correspondence between the  $G$  orbits of ordered pairs of the set  $\mathbf{P}$  and the double cosets of the decomposition

$$G = F_1 \cup F_1g_2F_1 \cup \dots \cup F_1g_jF_1 \cup \dots \cup F_1g_qF_1, \quad j = 1, 2, \dots, q. \quad (3.2.3.100)$$

$$G(\mathbf{S}_1, \mathbf{S}_j) \leftrightarrow F_1g_jF_1 \text{ where } \mathbf{S}_j = g_j\mathbf{S}_1. \quad (3.2.3.101)$$

This bijection allows one to express the partition of the set  $\mathbf{P}$  of all ordered pairs into  $G$  orbits,

$$\mathbf{P} = G(\mathbf{S}_1, \mathbf{S}_1) \cup G(\mathbf{S}_1, g_2\mathbf{S}_1) \cup \dots \cup (\mathbf{S}_1, \mathbf{S}_j) \cup \dots \cup G(\mathbf{S}_1, g_q\mathbf{S}_1), \quad (3.2.3.102)$$

where  $\{g_1 = e, g_2, \dots, g_j, \dots, g_q\}$  is the set of representatives of double cosets in the decomposition (3.2.3.100) (Janovec, 1972).

Proposition 3.2.3.35 applies directly to pairs of domain states (domain pairs) and allows one to find transposition laws that can appear in the low-symmetry phase (see Section 3.4.3).

For more details and other applications of group action see *e.g.* Kopský (1983), Lang (1965), Michel (1980), Opechowski (1986), Robinson (1982), and especially Kerber (1991, 1999).

#### References

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