

3.2. TWINNING AND DOMAIN STRUCTURES

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,

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

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

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

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

$$\mathbf{r}' = x'_1\mathbf{e}_1 + x'_2\mathbf{e}_2 + x'_3\mathbf{e}_3. \quad (3.2.3.42)$$

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

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

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

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

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 $E(3)$,

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

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 S_i, S_j, S_k, \dots and $\varphi : G \times A \rightarrow A$ a mapping that assigns to an ordered pair (g, S_i) , where $g \in G, S_i$ and S_i are objects of the set A :

$$\varphi : (g, S_i) \mapsto S_k, \quad g \in G, \quad S_i, S_k \in A. \quad (3.2.3.46)$$

The ordered pair (g, S_i) can often be written simply as a product gS_i and the mapping as an equation. Then the relation (3.2.3.46) can be expressed in a simpler form:

$$gS_i = S_k, \quad g \in G, \quad S_i, S_k \in A. \quad (3.2.3.47)$$

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

$$eS_i = S_i \text{ for any } S_i \in A, \quad (3.2.3.48)$$

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

$$h(gS_i) = (hg)S_i \text{ for any } h, g \in G \text{ and any } S_i \in A, \quad (3.2.3.49)$$

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 $gS_i = S_k$ followed by the second action $hS_k = S_m$ gives the same result as if one first calculates the product $hg = p$ and then applies it to S_i , $pS_i = S_m$.

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 $\mathbf{a}'_1, \mathbf{a}'_2, \mathbf{a}'_3$,

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

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 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

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space. At constant temperature and external fields, the states are in one-to-one correspondence with the orientations of the crystal.

Application of an isometry on a state of a crystal can be treated as a group action: Let G be a point group and \mathbf{A} a set of all conceivable states of a crystal. We denote by \mathbf{S}_i the state of the crystal in an initial orientation. An operation g of G changes the orientation of the crystal and the resulting state \mathbf{S}_k of the crystal in a new orientation is determined by \mathbf{S}_i and g . This is, in mathematical terms, a mapping of a pair (g, \mathbf{S}_i) on a state \mathbf{S}_k from the set \mathbf{A} , $\varphi : (g, \mathbf{S}_i) \mapsto \mathbf{S}_k$, or in the shorthand notation,

$$g\mathbf{S}_i = \mathbf{S}_k, \quad g \in G, \quad \mathbf{S}_i, \mathbf{S}_k \in \mathbf{A}. \quad (3.2.3.51)$$

Since this mapping fulfils conditions (3.2.3.48) and (3.2.3.49), it is a group action. We note that for some g the resulting state \mathbf{S}_k can be identical with the initial state \mathbf{S}_i and that several operations can produce the same resulting state \mathbf{S}_k .

Group action of an isometry on a crystal applies in a natural way to domain structures, where the group G describes the symmetry of the parent (high-symmetry) phase and the states $\mathbf{S}_i, \mathbf{S}_k$ are crystallographically equivalent (G -equivalent) states of the distorted (low-symmetry) phase called *domain states*. This means that domain states are states that are crystallographically equivalent in G . In a continuum description, domain states differ in orientation and are called *ferroic domain states* or orientation states (see Section 3.4.3.2).

Example [aT] 3.2.3.10. Let us consider a property tensor τ (e.g. polarization, permittivity, piezoelectric coefficients) and let us denote by $\tau^{(i)}$ components of this tensor expressed in a fixed reference coordinate system. This set can be represented by a point in the corresponding tensor space. Let us denote by \mathbf{B} the set of all points of this tensor space and by G a point group. The mapping

$$g\tau^{(i)} = \tau^{(k)}, \quad g \in G, \quad \tau^{(i)}, \tau^{(k)} \in \mathbf{B}, \quad (3.2.3.52)$$

is defined by the transformation law of the tensor components (see Chapter 1.1). This mapping fulfils conditions (3.2.3.48) and (3.2.3.49), and can therefore be treated as a group action.

Example [aS] 3.2.3.11. Let G be a group, F a subgroup of G , $F \subset G$, and \mathbf{C} the set of all subgroups of G . The group G can act on the set \mathbf{C} by conjugation:

$$\varphi : (g, F) \mapsto gFg^{-1}, \quad g \in G, F \in \mathbf{C}. \quad (3.2.3.53)$$

In this case, one has to write the mapping explicitly since the abbreviated form gF would mean a left coset and not a conjugate subgroup gFg^{-1} . One also has to corroborate the validity of condition (3.2.3.49): $(h, (g, F)) \mapsto (h, (gFg^{-1})) \mapsto h(gFg^{-1})h^{-1} = hgF(hg)^{-1}$, which is the image of $((hg), F)$.

An action of a group G on a set \mathbf{A} introduces two basic notions, namely stabilizers and orbits.

3.2.3.3.2. Stabilizers (isotropy groups)

The concept of a stabilizer is closely connected with the notion of the symmetry group of an object. Under the *symmetry group* F of an object \mathbf{S} one understands the set of all operations (isometries) that map the object onto itself, i.e. leave this object \mathbf{S} invariant. In this approach, one usually ‘attaches’ the symmetry elements to the object. Then the symmetry group F of the object is its inherent property which does not depend on the orientation and position of the object in space. The term *eigensymmetry* is used in Chapter 3.3 for symmetry groups defined in this way.

The notion of a stabilizer describes the symmetry properties of an object from another standpoint, in which the object and the group of isometries are decoupled and introduced independently. One chooses a reference coordinate system and a group G of isometries, the operations of which have a defined orientation in this reference system. Usually, it is convenient to choose as the reference system the standard coordinate system (crystallographic or crystallophysical) of the group G . The object \mathbf{S}_i under consideration is specified not only *per se* but also by its orientation in the reference system. Those operations of G that map the object in this orientation onto itself form a group called the stabilizer of \mathbf{S}_i in the group G . An algebraic definition is formulated in the following way:

Definition [s] 3.2.3.12. The *stabilizer (isotropy group)* $I_G(\mathbf{S}_i)$ of an object \mathbf{S}_i of a G -set \mathbf{A} in group G is that subgroup of G comprised of all operations of G that do not change \mathbf{S}_i ,

$$I_G(\mathbf{S}_i) = \{g \in G | g\mathbf{S}_i = \mathbf{S}_i\}, \quad g \in G, \quad \mathbf{S}_i \in \mathbf{A}. \quad (3.2.3.54)$$

Unlike the ‘eigensymmetry’, the stabilizer $I_G(\mathbf{S}_i)$ depends on the group G , is generally a subgroup of G , $I_G(\mathbf{S}_i) \subseteq G$, and may change with the orientation of the object \mathbf{S}_i .

There is an important relation between stabilizers of two objects from a G -set (see e.g. Aizu, 1970; Kerber, 1991):

Proposition 3.2.3.13. Consider two objects $\mathbf{S}_i, \mathbf{S}_k$ from a G -set related by an operation g from the group G . The respective stabilizers $I_G(\mathbf{S}_i), I_G(\mathbf{S}_k)$ are conjugate by the same operation g ,

$$\text{if } \mathbf{S}_k = g\mathbf{S}_i, \text{ then } I_G(\mathbf{S}_k) = gI_G(\mathbf{S}_i)g^{-1}. \quad (3.2.3.55)$$

Let us illustrate the meaning of stabilizers with four examples of group action considered above.

Example [sP] 3.2.3.14. Let \mathcal{G} be a crystallographic space group and X a point of the three-dimensional point space $E(3)$ (see Example 3.2.3.7). The stabilizer $\mathcal{I}_{\mathcal{G}}(X)$, called the *site-symmetry group* of the point X in \mathcal{G} , consists of all symmetry operations of \mathcal{G} that leave the point X invariant. Consequently, the stabilizer $\mathcal{I}_{\mathcal{G}}(X)$ is a crystallographic point group. If the stabilizer $\mathcal{I}_{\mathcal{G}}(X)$ consists only of the identity operation, then the point X is called a *point of general position*. If $\mathcal{I}_{\mathcal{G}}(X)$ is a non-trivial point group, X is called a *point of special position* (IT A, 2002).

Example [sC] 3.2.3.15. The symmetry of domain states $\mathbf{S}_i, \mathbf{S}_k, \dots$, treated in Example [sP] 3.2.3.9, is adequately expressed by their stabilizers in the group G of the parent (high-symmetry) phase, $I_G(\mathbf{S}_i) = F_i, I_G(\mathbf{S}_k) = F_k, \dots$. These groups are called *symmetry groups of domain states*. If domain states $\mathbf{S}_i, \mathbf{S}_k$ are related by an operation $g \in G$, then their symmetry groups are, according to (3.2.3.55), conjugate by g ,

$$\text{if } \mathbf{S}_k = g\mathbf{S}_i \text{ then } F_k = gF_i g^{-1}. \quad (3.2.3.56)$$

Symmetry characterization of domain states by their stabilizers properly reflects a difference between ferroelastic single domain states and ferroelastic disoriented domain states (see Sections 3.4.3 and 3.4.4).

Example [sT] 3.2.3.16. The notion of the stabilizer enables one to formulate a basic relation between the symmetry group of the parent phase, the symmetry group of the first domain state \mathbf{S}_1 and order parameters of the transition. In a microscopic description, the symmetry of the parent phase is described by a space group \mathcal{G} and the symmetry of the first basic (microscopic) single domain

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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 GS_i , is a set of all objects of \mathbf{A} that are G -equivalent with \mathbf{S}_i ,

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

Important note: The object \mathbf{S}_i of the orbit GS_i is called the *representative of the orbit* GS_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 GS_r, GS_s of a G -set \mathbf{A} are either identical or disjoint. The set \mathbf{A} can therefore be partitioned into disjoint orbits,

$$\mathbf{A} = GS_i \cup GS_k \cup \dots \cup GS_q. \quad (3.2.3.63)$$

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 a *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 GS_1 , where G is the parent phase symmetry, assembles all G -equivalent domain states,

$$GS_1 = \{\mathbf{S}_1, \mathbf{S}_2, \dots, \mathbf{S}_n\}. \quad (3.2.3.64)$$

The existence of several equivalent states is the main characteristic feature of domain states. Domain states of the orbit GS_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 GS_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 GS_i constitute the orbit (3.2.3.66) of all subgroups conjugate under G . One can thus associate with each orbit GS_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 GS_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-

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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 $G X_1$ 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 (3×3) 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 λ ,

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

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 φ 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).

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