

3.2. Twinning and domain structures

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3.2.1. Introduction and history

Twins have been known for as long as mankind has collected minerals, admired their beauty and displayed them in museums and mineral collections. In particular, large specimens of contact and penetration twins with their characteristic re-entrant angles and simulated higher symmetries have caught the attention of mineral collectors, miners and scientists. *Twinning* as a special feature of crystal morphology, therefore, is a ‘child’ of mineralogy, and the terms and symbols in use for twinned crystals have developed during several centuries together with the development of mineralogy.

The first scientific description of *twinning*, based on the observation of re-entrant angles, goes back to Romé de l’Isle (1783). Haüy (1801) introduced symmetry considerations into twinning. He described *hemitropes* (twofold rotation twins) and *penetration twins*, and stated that the *twin face* is parallel to a possible crystal face. Much pioneering work was done by Weiss (1809, 1814, 1817/1818) and Mohs (1822/1824, 1823), who extended the symmetry laws of twinning and analysed the symmetry relations of many twins occurring in minerals. Naumann (1830) was the first to distinguish between twins with parallel axes (*Zwillinge mit parallelen Achsensystemen*) and twins with inclined (*crossed*) axes (*Zwillinge mit gekreuzten Achsensystemen*), and developed the mathematical theory of twins (Naumann, 1856). A comprehensive survey of the development of the concept and understanding of twinning up to 1869 is presented by Klein (1869).

At the beginning of the 20th century, several important mineralogical schools developed new and far-reaching ideas on twinning. The French school of Mallard (1879) and Friedel (1904) applied the lattice concept of Bravais to twinning. This culminated in the lattice classification of twins by Friedel (1904, 1926) and his introduction of the terms *macles par méridrie* (twinning by merohedry), *macles par pseudo-méridrie* (twinning by pseudo-merohedry), *macles par méridrie réticulaire* [twinning by reticular (lattice) merohedry] and *macles par pseudo-méridrie réticulaire* (twinning by reticular pseudo-merohedry). This concept of twinning was very soon taken up and further developed by Niggli in Zürich, especially in his textbooks (1919, 1920, 1924, 1941). The lattice theory of Mallard and Friedel was subsequently extensively applied and further extended by J. D. H. Donnay (1940), and in many later papers by Donnay & Donnay, especially Donnay & Donnay (1974). The Viennese school of Tschermak (1904, 1906), Tschermak & Becke (1915), and Tertsch (1936) thoroughly analysed the morphology of twins, introduced the *Kantennormalengesetz* and established the minimal conditions for twinning. The structural and energy aspects of twins and their boundaries were first accentuated and developed by Buerger (1945). Presently, twinning plays an important (but negative) role in crystal structure determination. Several sophisticated computer programs have been developed that correct for the presence of twinning in a small single crystal.

A comprehensive review of twinning is given by Cahn (1954); an extensive treatment of mechanical twinning is presented in the monograph by Klassen-Neklyudova (1964). A tensor classification of twinning was recently presented by Wadhawan (1997, 2000). Brief modern surveys are contained in the textbooks by Bloss (1971), Giacomazzo (1992) and Indenbom (see Vainshtein *et al.*, 1995), the latter mainly devoted to theoretical aspects. In previous volumes of *International Tables*, two articles on twinning

have appeared: formulae for the calculation of characteristic twin data, based on the work by Friedel (1926, pp. 245–252), are collected by Donnay & Donnay in Section 3 of Volume II of the previous series (Donnay & Donnay, 1972), and a more mathematical survey is presented by Koch in Chapter 1.3 of Volume C of the present series (Koch, 1999).

Independently from the development of the concept of twinning in mineralogy and crystallography, summarized above, the concept of *domain structures* was developed in physics at the beginning of the 20th century. This started with the study of *ferromagnetism* by Weiss (1907), who put forward the idea of a molecular field and formulated the hypothesis of differently magnetized regions, called *ferromagnetic domains*, that can be switched by an external magnetic field. Much later, von Hámos & Thiessen (1931) succeeded in visualizing magnetic domains by means of colloidal magnetic powder. For more details about magnetic domains see Section 1.6.4 of the present volume.

In 1921, Valasek (1921) observed unusual dielectric behaviour in Rochelle salt and pointed out its similarity with anomalous properties of ferromagnetic materials. This analogy led to a prediction of ‘electric’ domains, *i.e.* regions with different directions of spontaneous polarization that can be switched by an electric field. Materials with this property were called *Seignette electrics* (derived from the French, ‘*sel de Seignette*’, denoting Rochelle salt). The term *seignettelectrics* is still used in Russian, but in English has been replaced by the term *ferroelectrics* (Mueller, 1935). Although many experimental and theoretical results gave indirect evidence for *ferroelectric domain structure* [for an early history see Cady (1946)], it was not until 1944 that Zwicker & Scherrer (1944) reported the first direct optical observation of the domain structure in ferroelectric potassium dihydrogen phosphate (KDP). Four years later, Klassen-Neklyudova *et al.* (1948) observed the domain structure of Rochelle salt in a polarizing microscope (see Klassen-Neklyudova, 1964, p. 27). In the same year, Blattner *et al.* (1948), Kay (1948) and Matthias & von Hippel (1948) visualized domains and domain walls in barium titanate crystals using the same technique.

These early studies also gave direct evidence of the influence of mechanical stress and electric field on domain structure. Further, it was disclosed that a domain structure exists only below a certain temperature, called the *Curie point*, and that the crystal structures below and above the Curie point have different point-group symmetries. The Curie point thus marks a structural phase transition between a *paraelectric phase* without a domain structure and a *ferroelectric phase* with a ferroelectric domain structure. Later, the term ‘Curie point’ was replaced by the more suitable expression *Curie temperature* or *transition temperature*.

The fundamental achievement in understanding phase transitions in crystals is the *Landau theory* of continuous phase transitions (Landau, 1937). Besides a thermodynamic explanation of anomalies near phase transitions, it discloses that any continuous phase transition is accompanied by a discontinuous decrease of crystal symmetry. In consequence, a phase with lower symmetry can always form a domain structure.

The basic role of symmetry was demonstrated in the pioneering work of Zheludev & Shuvalov (1956), who derived by simple crystallographic considerations the point groups of paraelectric and ferroelectric phases of all possible ferroelectric phase transitions and gave a formula for the number of ferroelectric domain states.

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A mechanical analogy to ferroelectric domains exists in the form of domains that differ in strain and can be switched by mechanical stress. This effect was studied under the name 'twinning with change of form' in the monoclinic ferroelectric phase of Rochelle salt by Klassen-Neklyudova *et al.* (1948) and Chernysheva (1950). A detailed description of this work in English is presented by Klassen-Neklyudova (1964, pp. 27–30, 75–78) in her monograph on mechanical twinning of crystals. Indenbom (1960) has shown that such behaviour is not confined to ferroelectric crystals and has listed many symmetry changes of potential phase transitions accompanied by the appearance of a spontaneous strain that could give rise to domains with different strain. Aizu (1969) called such crystals *ferroelastic crystals* in analogy with ferroelectric crystals. *Ferroelastic domains* differ in spontaneous strain and can be switched by mechanical stress.

Generalization of the concepts of ferromagnetic, ferroelectric and ferroelastic crystals followed soon after (Aizu, 1970): A *ferroic crystal* has two or more *orientation states* (oriented bulk structures of domains) that can be switched by means of a magnetic field, an electric field, a mechanical stress or by a combination of these. *Ferroic domains* are distinct in some tensors describing the material properties of the crystal. Aizu has also shown that the type of domain structure is determined by the change of point-group symmetry at the structural phase transition from a *prototypic (parent, high-symmetry) phase* without domains to a *ferroic (distorted, low-symmetry, daughter) phase* in which domains appear.

A more detailed history of the research of ferromagnetic, ferroelectric, ferroelastic and ferroic materials in general can be found in the book by Wadhawan (2000).

The domain structure determines to a certain extent electric, elastic, electromechanical and other properties of ferroic crystals. The investigation of domain structures has thus become an inseparable part of the research of ferroelectrics, ferroelastics and ferroic crystalline materials in general.

Most of the work has been devoted to ferroelectrics, since their specific properties have found important applications, some of which (*e.g.* production of anisotropic ceramics, ferroelectric memories) are based on irreversible and hysteretic changes of the ferroelectric domain structure under an electric field. References to ferroelectric, ferroelastic and other domain structures are given at the end of Section 3.4.1.

Even though the basic concepts of *twinning* and *domain structures* are closely related and have many aspects in common, the study of both subjects has developed independently, using different terms and symbols to describe rather similar facts. There are many cases that can be treated equally well by both approaches, *e.g.* merohedral twins and non-ferroelastic domain structures. There are cases, however, which can only be understood with one of the two concepts, *e.g.* the (111) spinel twins cannot be interpreted as a domain structure, because a high-symmetry parent phase does not exist. Of the two topics, twinning is the older, whereas the younger topic domain structure has recently advanced to a more detailed physical understanding.

In the two following chapters, 3.3 and 3.4, the two topics are treated separately and in their own right. It will be apparent that the two approaches, despite the great similarity of their objects, are quite different: for *domain structures* the all-important theoretical basis is the existence of a – real or potential (hypothetical) – *parent (prototypic) phase* from which the *ferroic (distorted) phase* is derived. This lowering of symmetry, expressed by a group–subgroup relation between the symmetries of the parent and ferroic phases, is the source of an impressive theoretical edifice which allows the explanation, and even the prediction, of many crystallographic properties of a given domain structure.

The situation is different in *twinning*: whereas *transformation twins* are closely related to domain structures and hence can be treated with the same theoretical tools, many *growth twins* and

mechanical twins are characterized by the absence of an existing – and even a hypothetical – parent structure. From this it follows that growth and mechanical twins (which are the typical twin specimens of mineral collections) are to a much lesser extent amenable to group-theoretical analysis. Instead, each twinning case must be considered separately, and the orientation and contact relations of the twin partners must be individually ascertained. This requires discussion of many 'type cases'.

The present chapter continues with a short excursion into bicrystallography (Section 3.2.2), a topic not treated further in this article, followed by Section 3.2.3 with an exposition of basic concepts of set theory and group theory needed in Chapters 3.3 and 3.4.

3.2.2. A brief survey of bicrystallography

Both twinning and domain structures appear to be special cases of the relatively young research field of *bicrystallography* (Pond & Vlachavas, 1983), which has its origin in the study of *grain boundaries* in metals. Grains are coexisting crystals with identical composition and structure but with different orientations. Coexisting grains can be formally treated as generalized twins in which one of the conditions (*viz* a crystallographic relation between the twin components) is dropped.

A common feature of twins, domain structures and grain aggregates is the interface between coexisting crystals. The simplest edifice containing a crystalline interface is a bicrystal consisting of two semi-infinite perfect crystals (components) and a single planar interface along which the two crystals adjoin. For easier comprehension, one crystal of a bicrystal can be 'coloured' black and the other crystal white. Then the operations that leave both crystals unchanged are trivial colour-preserving symmetry operations, whereas the *symmetrizing operations*, which transform the black crystal into the white one and *vice versa*, are nontrivial colour-reversing operations. If one marks these colour-reversing operations by a prime or a star, then the symmetry group of a bicrystal has the structure of a *dichromatic (black-and-white) group* (see Section 3.2.3.2.7).

The dissymmetrization (symmetry reduction or lowering, symmetry descent) plays a basic role in bicrystallography. This is a process in which an object changes from a high-symmetry form into a low-symmetry form. As shown in Chapter 3.4, any dissymmetrization is accompanied by the formation of several symmetrically equivalent specimens of the low symmetry called *variants*. Variants are related by suppressed (lost) symmetry operations that are present in the low-symmetry form but are missing in the high-symmetry form. The set of all low-symmetry variants recovers the symmetry of the high-symmetry form. This general statement is referred to as the *law of symmetry compensation* and can be alternatively expressed by the following sentence (Shubnikov & Koptsik, 1974): If symmetry is reduced at one structural level, it arises and is recovered at another structural level. A paradigmatic example of dissymmetrization is a structural phase transition in which a high-symmetry parent (prototypic) phase changes into a low-symmetry distorted (ferroic) phase. The variants of the low-symmetry distorted phase are called single domain states or orientation states. The set of all single domain states recovers the high symmetry of the parent phase (see Chapter 3.4).

A systematic method for deriving the bicrystal symmetry, which is identical with the symmetry of the bicrystal interface, consists of four hierarchical stages (Pond & Vlachavas, 1983). At each stage, the bicrystal is represented by a construct (model) which is more detailed – and has, therefore, the same or lower symmetry – than the construct of the previous stage. These successive dissymmetrizations bring about at each stage equivalent variants of the bicrystal's construct. Different sets of variants

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at different stages have distinct physical significance and provide a basic generic classification of bicrystals and their interfaces.

The first stage deals with the so-called dichromatic pattern consisting of two interpenetrating black and white lattices of the two crystal components (Pond & Bollmann, 1979). The coinciding 'grey' points constitute the *coincidence site lattice* (CSL) (see Bollmann, 1970, 1982), which corresponds to the twin lattice in twinning (see Section 3.3.8). To find variants of the dichromatic pattern, bicrystallography replaces the symmetry group of a nonexistent previous 'zero stage' with a minimal group containing symmetries of the black crystal and the white crystal. This group is called the *embracing* or *fundamental group of dichromatic patterns* (Shubnikov & Koptsik, 1974; Pond & Vlachavas, 1983; Wadhawan, 2000). If the symmetry group of the dichromatic pattern is smaller than the embracing group, then this dissymmetrization produces orientational or translational variants of the dichromatic pattern.

In the second stage, black and white lattices are decorated by atoms and these crystal structures are represented by lattice complexes. [A lattice complex of a crystal is here defined as the set of points obtained by carrying out on each occupied atomic position all symmetry operations of the crystal's space group. Note that in crystallography the term 'lattice complex' has a different meaning; see *IT A* (2002), Parts 8 and 14.] Two interpenetrating black and white lattice complexes of crystal components form the dichromatic complex of a bicrystal. If the symmetry of the dichromatic complex is lower than that of the dichromatic pattern, the dissymmetrization gives rise to complex variants of the dichromatic complex. The concept of a dichromatic complex corresponds to the concept of a domain pair in domain structure analysis (see Section 3.4.3).

Mental constructions of the first two stages specify only the relation between the lattices and structures of crystal components of a bicrystal. In the third stage, an *ideal bicrystal* is formed by sectioning the black-and-white lattice (or structure) on the interface plane and discarding the black lattice (or structure) on one side of the section and the white lattice (structure) on the other side. If the interfacial plane is a crystallographic plane with two-dimensional periodicity, then the symmetry of this ideal bicrystal is described by a *dichromatic layer group* (see Sections 3.4.4.2 and 3.4.4.3). This group is smaller than the space-group symmetry of the dichromatic complex and this dissymmetrization gives rise to *morphological variants* of the ideal bicrystal. Operations suppressed at this dissymmetrization relate different morphological variants of the ideal bicrystal. An ideal bicrystal corresponds to a domain twin with zero-thickness domain wall (see Section 3.4.4).

All three preceding stages use geometrical models of an interface with fixed atomic positions. At the final fourth stage, these geometrical constraints are lifted and the ideal bicrystal relaxes to a *real* or *relaxed bicrystal* with a minimum free energy. During this relaxation process the interface plane may migrate into either crystal, one crystal may translate rigidly with respect to the other, and each atom may adjust its position to relax any resultant force acting on it. The relaxation may even include insertion or removal of additional material at the interface. If the symmetry of the relaxed bicrystal is lower than that of the ideal bicrystal, then relaxational variants of the relaxed bicrystal appear. The one-dimensional interface between two interfacial relaxational variants forms a line defect of the bicrystal interface. Relaxation variants of finite-thickness domain walls and line defects in these walls are discussed in Section 3.4.4.

Two main theoretical approaches have been used in examining the microscopic structure of a real bicrystal interface. In the older one, a real interface is treated as a *periodic array of dislocations*. This approach, still based on geometrical models, has explained successfully the microscopic structure of small-angle grain boundaries, but has failed in large-angle grain boundaries (misorientation angle larger than 15°).

More recent investigations utilizing computer simulations allow one to lift geometrical constraints and permit the calculation of equilibrium atomic positions directly from interatomic forces. These calculations have revealed that the lattice coincidence is almost always lost upon relaxation and that the microscopic structure of bicrystal interfaces can be described as an ordered sequence of coordination polyhedra. These conclusions have been confirmed by high-resolution electron microscopy. For more details see, for example, Fischmeister (1985), Sutton & Balluffi (1995) and Gottstein & Shvindlerman (1999).

The first three 'classical' stages of the bicrystallographical analysis already yield valuable conclusions. They disclose generic relations between different interfaces, specify crystallographically equivalent variants of an interface and classify line defects in interfaces. The symmetry of a bicrystal imposes constraints on tensor properties of the bicrystal interface, provides classification of the interfacial vibrational modes, discloses possible interfacial transitions *etc.* (see, for example, Kalonji, 1985).

The methodology of bicrystallography has many common features with the symmetry analysis of domain structures but, since both approaches have developed independently, they use a different terminology. Moreover, in comparison with bicrystals, domain structures and twins are more restricted by crystallographic constraints. This has resulted in more extensive application of group theory in domain structures than in bicrystallography. On the other hand, bicrystallography is more general and can even treat interfaces between two crystals belonging to different phases (heterophase interfaces).

A synoptic 'roadmap for the use of interfacial symmetry', compiled by Kalonji (1985), provides a quick guide to the possible applications of bicrystallography. A short introduction to bicrystallography can be found in Wadhawan (2000); a brief comparison of the concepts and terminologies of bicrystals, twins and domain structures is presented by Hahn *et al.* (1999). An extensive treatment of bicrystallography is available in the paper by Pond & Vlachavas (1983) and in the book by Sutton & Balluffi (1995), where other aspects of crystalline interfaces are also thoroughly covered.

3.2.3. Mathematical tools

Analysis of domain structures and twins does not deal primarily with single-crystal structures, as does classical crystallography, but studies collections of several crystal structures – which usually differ in orientation and position in space – and examines relations between these structures and their coexistence. The exact formulation of such an analysis uses mathematical concepts that are not yet quite common in crystallography. Thus, *e.g.*, a collection of crystallographic objects has to be decomposed into equivalence classes called orbits and strata, or the symmetry of an object (structure, domain wall, twin) has to be described with respect to a given group, which necessitates replacing the usual notion of a symmetry group by a 'stabilizer' (isotropy group). A prerequisite of introducing these terms is the concept of group action, which provides a basic and efficient tool for domain-structure analysis.

Another special feature of domain studies is that one can associate with a ferroic structure under study another structure, called the parent (prototypic) structure, from which the ferroic structure can be derived by small microscopic distortions. The fact that the symmetry of the ferroic phase is lower than that of the parent phase invokes the notion of a subgroup. Associated notions such as conjugate subgroups, normalizers and decomposition of a group into left and double cosets of a subgroup play an important role in the analysis.

Since some of these concepts are not available in standard texts, we present in this section the necessary mathematical

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background and explanation of terms and relations that appear in Chapters 3.3 and 3.4.

Section 3.2.3.1 introduces the basic concepts of set theory and explains the notion of unordered and ordered pairs, mappings of sets and the partition of a set into equivalence classes. Section 3.2.3.2 deals with basic group theory and is devoted mainly to group–subgroup relations and relevant notions, of which the coset decompositions are of central importance. In Section 3.2.3.3, group theory is combined with set theory in the ‘action of a group on a set’ (for short, ‘group action’). Notions of stabilizer, orbit and stratum are explained and their significance is illustrated by several examples.

A simple exposition of the main group-theoretical concepts, including group action and orbits, can be found in the book by Hahn & Wondratschek (1994). A concise presentation of group actions and related notions with many examples has been given by Michel (1980). Other more detailed references are given at the end of each of the following sections.

3.2.3.1. Sets, pairs, mappings and equivalence classes

3.2.3.1.1. Sets

Definition 3.2.3.1. A set is a collection of distinguishable objects. The objects constituting a set are called *elements* (or *points*) of the set.

In Chapter 3.4 we encounter mainly two types of sets: sets the elements of which are crystalline objects (domain states, domain twins, domain walls *etc.*), and sets, like groups, with elements of mathematical nature, *e.g.* rotations, transformations, operations *etc.* The sets of crystalline objects will be denoted by capital sans-serif letters, *e.g.* $\mathbf{A}, \mathbf{B}, \dots$, and capital bold letters, *e.g.* $\mathbf{S}, \mathbf{M}, \mathbf{N}, \dots$ or $\mathbf{S}_1, \mathbf{S}_2, \mathbf{S}_3, \dots$, will be used to denote elements of such sets. Groups will be denoted by capital italic letters, *e.g.* G, F *etc.*, and their elements by lower-case italic letters, *e.g.* g, h, \dots . The exposition of this section is given for sets the elements of which are (crystalline) objects, but all notions and relations hold for any other sets.

If an element \mathbf{S} belongs to the set \mathbf{A} , one writes $\mathbf{S} \in \mathbf{A}$, in the opposite case $\mathbf{S} \notin \mathbf{A}$. Sets consisting of a small number of elements can be expressed explicitly by writing their elements between curly braces, $\mathbf{A} = \{\mathbf{S}, \mathbf{M}, \mathbf{N}, \mathbf{Q}\}$. The order of elements in the symbol of the set is irrelevant. From the definition of a set it follows that there are no equal elements in the set, or in other words, any two equal elements coalesce into one:

$$\{\mathbf{S}, \mathbf{S}\} = \{\mathbf{S}\}. \quad (3.2.3.1)$$

If a set contains many (or an infinite number of) elements, the elements are specified in another way, *e.g.* by stating that they have a certain property in common.

The number of elements in a set is the *order of the set*. A *finite set* \mathbf{A} consists of a finite number of elements and this number is denoted by $|\mathbf{A}|$. An *infinite set* contains infinite number of elements and an *empty set*, denoted by \emptyset , contains no element. In what follows, the term ‘set’ will mean a ‘finite nonempty set’ unless explicitly stated otherwise.

A set \mathbf{B} is a *subset* of \mathbf{A} , $\mathbf{B} \subseteq \mathbf{A}$ or $\mathbf{A} \supseteq \mathbf{B}$, if every element of \mathbf{B} is an element of \mathbf{A} . If each element of \mathbf{B} is an element of \mathbf{A} , and *vice versa*, then \mathbf{B} is *equal to* or *identical with* \mathbf{A} , $\mathbf{B} = \mathbf{A}$ or $\mathbf{A} = \mathbf{B}$. If there exists at least one element of \mathbf{A} which is not contained in \mathbf{B} , then \mathbf{B} is a *proper subset* of \mathbf{A} , $\mathbf{B} \subset \mathbf{A}$ or $\mathbf{A} \supset \mathbf{B}$. The subset \mathbf{B} is often defined by a restriction that specifies only some elements of \mathbf{A} as elements of \mathbf{B} . This is written in short as $\mathbf{B} = \{\mathbf{S} \in \mathbf{A} | \text{restriction on } \mathbf{S}\}$; the expression means that \mathbf{B} consists of *all* elements of \mathbf{A} that satisfy the restriction given behind the sign $|$.

The *intersection* of two sets \mathbf{A} and \mathbf{B} , $\mathbf{A} \cap \mathbf{B}$ or $\mathbf{B} \cap \mathbf{A}$, is a set comprising all elements that belong both to \mathbf{A} and to \mathbf{B} . If the sets

\mathbf{A} and \mathbf{B} have no element in common, $\mathbf{A} \cap \mathbf{B} = \emptyset$, then one says that the sets \mathbf{A} and \mathbf{B} are *disjoint*. The *union of sets* \mathbf{A} and \mathbf{B} , $\mathbf{A} \cup \mathbf{B}$ or $\mathbf{B} \cup \mathbf{A}$, is a set consisting of all elements that belong either to \mathbf{A} or to \mathbf{B} . Sometimes the symbol $+$ is used instead of the symbol \cup . The *difference of set* \mathbf{A} and \mathbf{B} , or the *complement of* \mathbf{B} *in* \mathbf{A} , $\mathbf{A} - \mathbf{B}$, comprises those elements of \mathbf{A} that do not belong to \mathbf{B} .

3.2.3.1.2. Pairs

A collection of two objects \mathbf{S}_i and \mathbf{S}_k constitutes an *unordered pair*. The objects of an unordered pair are called *elements* or *points*. A *trivial unordered pair* consists of two identical elements. A non-trivial unordered domain pair comprises two non-identical elements and is identical with a set of order two.

Note that we do not identify an unordered pair with a set of order two where, according to (3.2.3.1), two equal objects coalesce into one. In spite of this difference we shall use the same symbol for the unordered pair as for the set of order two, but reverse the symbol $\{\mathbf{S}, \mathbf{S}\}$ for the trivial unordered pair. With this reservation, the identity

$$\{\mathbf{S}_i, \mathbf{S}_k\} = \{\mathbf{S}_k, \mathbf{S}_i\} \quad (3.2.3.2)$$

holds for both unordered pairs and for sets of order two.

An *ordered pair*, denoted $(\mathbf{S}_i, \mathbf{S}_k)$, consists of the *first* and the *second member* of the pair. If $\mathbf{S}_i = \mathbf{S}_k$, the ordered pair is called a *trivial ordered pair*, $(\mathbf{S}_i, \mathbf{S}_i)$; if $\mathbf{S}_i \neq \mathbf{S}_k$ the pair $(\mathbf{S}_i, \mathbf{S}_k)$ is a *non-trivial ordered pair*. The ordered pair $(\mathbf{S}_k, \mathbf{S}_i)$ with a reversed order of elements is called a *transposed pair*. In contrast to unordered pairs, initial and transposed non-trivial ordered pairs are different objects,

$$(\mathbf{S}_i, \mathbf{S}_k) \neq (\mathbf{S}_k, \mathbf{S}_i) \text{ for } \mathbf{S}_i \neq \mathbf{S}_k. \quad (3.2.3.2a)$$

The members \mathbf{S}_i and \mathbf{S}_k of an ordered pair $(\mathbf{S}_i, \mathbf{S}_k)$ can either belong to one set, $\mathbf{S}_i \in \mathbf{A}, \mathbf{S}_k \in \mathbf{A}$, or each to a different set, $\mathbf{S}_i \in \mathbf{A}, \mathbf{S}_k \in \mathbf{B}$.

Two ordered pairs $(\mathbf{S}_i, \mathbf{S}_k)$ and $(\mathbf{S}_m, \mathbf{S}_p)$ are equal, $(\mathbf{S}_i, \mathbf{S}_k) = (\mathbf{S}_m, \mathbf{S}_p)$, if and only if $\mathbf{S}_i = \mathbf{S}_m$ and $\mathbf{S}_k = \mathbf{S}_p$.

We shall encounter ordered and unordered pairs in Sections 3.4.3 and 3.4.4, where the members of pairs are domain states or domain twins. However, pairs are also essential in introducing further concepts of set theory. The starting point is the following construction of a set of pairs that are formed from two sets:

A *Cartesian product* $\mathbf{A} \times \mathbf{B}$ of two sets \mathbf{A} and \mathbf{B} is a set of *all* ordered pairs (\mathbf{S}, \mathbf{M}) , where $\mathbf{S} \in \mathbf{A}, \mathbf{M} \in \mathbf{B}$. The sets \mathbf{A} and \mathbf{B} can be different or identical sets. If the sets \mathbf{A} and \mathbf{B} are finite, then the Cartesian product $\mathbf{A} \times \mathbf{B}$ consists of $|\mathbf{A}| \cdot |\mathbf{B}|$ ordered pairs.

3.2.3.1.3. Mappings

A *mapping* φ of a set \mathbf{A} into a set \mathbf{B} is a rule which assigns to each element $\mathbf{S} \in \mathbf{A}$ a unique element $\mathbf{M} \in \mathbf{B}$. This is written symbolically as $\varphi : \mathbf{S} \mapsto \mathbf{M}$ or $\mathbf{M} = \varphi(\mathbf{S})$, and one says that \mathbf{S} is mapped to \mathbf{M} under the mapping φ . The element \mathbf{M} is called the *image of the element* \mathbf{S} *under* φ . The assignment $\varphi : \mathbf{S} \mapsto \mathbf{M}$ can be expressed by an ordered pair (\mathbf{S}, \mathbf{M}) , if one ascribes \mathbf{S} to the first member of the pair and the element \mathbf{M} to the second member of the pair (\mathbf{S}, \mathbf{M}) . Then the mapping φ of a set \mathbf{A} into a set \mathbf{B} , symbolically written as $\varphi : \mathbf{A} \rightarrow \mathbf{B}$, can be identified with such a subset of ordered pairs of the Cartesian product $\mathbf{A} \times \mathbf{B}$ in which each element \mathbf{S} of \mathbf{A} occurs exactly once as the first member of the pair (\mathbf{S}, \mathbf{M}) . If \mathbf{A} is a finite set, then φ consists of $|\mathbf{A}|$ ordered pairs.

We note that in a mapping $\varphi : \mathbf{A} \rightarrow \mathbf{B}$ several elements of \mathbf{A} may be mapped to the same element of \mathbf{B} . In such a case, the mapping φ is called a *many-to-one mapping*. If the mapping $\varphi : \mathbf{A} \rightarrow \mathbf{B}$ is such that each element of \mathbf{B} is the image of some element of \mathbf{A} , then the mapping φ is called a *mapping of* \mathbf{A} *onto* \mathbf{B} . If φ is a mapping of \mathbf{A} onto \mathbf{B} and, moreover, each element of \mathbf{B} is

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the image of exactly one element of A , then the mapping φ becomes a *one-to-one correspondence between A and B* , $\varphi : A \leftrightarrow B$. In this case, A and B are of the same order.

One often encounters a situation in which one assigns to each ordered pair (S, M) an element N , where all three elements S, M, N are elements from the same set A , symbolically $\varphi : (S, M) \mapsto N$; $S, M, N \in A$ or $\varphi : A \times A \rightarrow A$. Such a mapping is called a *binary operation* or a *composition law* on the set A . A sum of two numbers $a + b = c$ or a product of two numbers $a \cdot b = c$, where a, b, c belong to the set of all real numbers, are elementary examples of binary operations.

3.2.3.1.4. Equivalence relation on a set, partition of a set

The notion of the ordered pair allows one to introduce another useful concept, namely the relation on a set. An example will illustrate this notion. Let \mathbb{Z} be a set of integers, $\mathbb{Z} = \{\dots, -2, -1, 0, 1, 2, \dots\}$. For each ordered pair (m, n) , $m, n \in \mathbb{Z}$, one can decide whether m is smaller than n , $m < n$, or not. All pairs (m, n) that fulfil the condition $m < n$ form a subset R of all possible ordered pairs $\mathbb{Z} \times \mathbb{Z}$. In other words, the relation $m < n$ defines a subset R of the set $\mathbb{Z} \times \mathbb{Z}$, $R \subset \mathbb{Z} \times \mathbb{Z}$. Similarly, the relation $|m| = |n|$ ($|n|$ denotes absolute value of n) defines another subset of $\mathbb{Z} \times \mathbb{Z}$.

To indicate that an element S is related to M by $\overset{R}{\sim}$, where $S, M \in A$, one writes $S \overset{R}{\sim} M$, where the relation R defines a subset R of all ordered pairs $A \times A$, $R \subset A \times A$ (the same letter R is used for the subset and for the relation on A). The opposite also holds: Each subset R of $A \times A$ defines a certain relation $\overset{R}{\sim}$ on A .

A relation $\overset{R}{\sim}$ is called an *equivalence relation on the set A* if it satisfies three conditions:

$$S \overset{R}{\sim} S \text{ for all } S \in A \text{ (reflexivity),} \quad (3.2.3.3)$$

$$\text{if } S, M \in A \text{ and } S \overset{R}{\sim} M, \text{ then } M \overset{R}{\sim} S \text{ (symmetry),} \quad (3.2.3.4)$$

$$\text{if } S, M, N \in A, S \overset{R}{\sim} M \text{ and } M \overset{R}{\sim} N, \text{ then } S \overset{R}{\sim} N \text{ (transitivity).} \quad (3.2.3.5)$$

Thus, for example, it is easy to corroborate that the relation $|m| = |n|$ on the set of integers \mathbb{Z} fulfils all three conditions (3.2.3.3) to (3.2.3.5) and is, therefore, an equivalence relation on the set \mathbb{Z} . On the other hand, the relation $m < n$ is not an equivalence relation on \mathbb{Z} since it fulfils neither the reflexivity (3.2.3.3) nor the symmetry condition (3.2.3.4).

Let $\overset{R}{\sim}$ be an equivalence relation on A and $S \in A$; all elements $M \in A$ such that $M \overset{R}{\sim} S$ constitute a subset of A denoted $[S]_R$ and called the *equivalence class of S with respect to $\overset{R}{\sim}$* (or the *R-equivalence class of S*). The element S is called the *representative* of the class $[S]_R$. Any other member of the class can be chosen as its representative. Any two elements of the equivalence class $[S]_R$ are *R-equivalent elements of A* .

From the definition of the equivalence class, it follows that any two elements $M, N \in A$ are either R-equivalent elements of A , $M \overset{R}{\sim} N$, and thus belong to the same class, $[M]_R = [N]_R$, or are not R-equivalent, and thus belong to two different classes that are disjoint, $[M]_R \cap [N]_R = \emptyset$. In this way, the equivalence relation $\overset{R}{\sim}$ divides the set A into disjoint subsets (equivalence classes), the union of which is equal to the set itself. Such a decomposition is called a *partition of the set A associated with the equivalence relation $\overset{R}{\sim}$* . For a finite set A this decomposition can be expressed as a union of equivalence classes,

$$A = [S]_R \cup [M]_R \cup \dots \cup [Q]_R, \quad (3.2.3.6)$$

where S, M, \dots, Q are representatives of the equivalence classes.

Generally, any decomposition of a set into a system of disjoint non-empty subsets such that every element of the set is a member of just one subset is called a *partition of the set*. To any partition of a set A there corresponds an equivalence relation $\overset{R}{\sim}$ such that the

R-equivalence classes of A form that partition. This equivalence relation defines two elements as equivalent if and only if they belong to the same subset.

The term ‘equivalent’ is often used when it is clear from the context what the relevant equivalence relation is. Similarly, the term ‘class’ is used instead of ‘equivalence class’. Sometimes equivalence classes have names that do not explicitly indicate that they are equivalence classes. For example, in group theory, conjugate subgroups, left, right and double cosets form equivalence classes (see Section 3.2.3.2). Often instead of the expression ‘partition of a set A ’ an equivalent expression ‘classification of the elements of a set A ’ is used. The most important equivalence classes in the symmetry analysis of domain structures are called orbits and will be discussed in Section 3.2.3.3.

More details on set theory can be found in Kuratowski & Mostowski (1968), Lipschutz (1981), and Opechowski (1986).

3.2.3.2. Groups and subgroups

3.2.3.2.1. Groups

Operations (isometries) that act on a body without changing its form and internal state combine in the same way as do elements of a group. Group theory is, therefore, the main mathematical tool for examining transformation properties – symmetry properties in particular – of crystalline objects. The basic concept of group theory is that of a group.

Definition 3.2.3.2. A *group G* is a set that satisfies four postulates:

(1) To each ordered pair (g_i, g_j) of two elements of G , there corresponds a unique element g_k of G , i.e. a binary operation (composition law) is defined on the set G . Usually, one writes the ordered pair simply as a ‘product’ $g_i g_j$ and the composition law as an equation,

$$g_i g_j = g_k, \quad g_i, g_j, g_k \in G. \quad (3.2.3.7)$$

This condition is referred to as *closure of G under multiplication*.

(2) The *multiplication is associative*, i.e. for any three elements g_i, g_j, g_k of G it holds that if $g_i g_j = g_l$ and $g_j g_k = g_m$ then $g_l g_k = g_i g_m$. This condition is usually written as one equation,

$$(g_i g_j) g_k = g_i (g_j g_k), \quad (3.2.3.8)$$

which expresses the requirement that the product of any three elements of G is the same, no matter which two of the three one multiplies first, as long as the order in which they stand is not changed. From postulate (2) it follows that the product of any finite sequence of group elements is determined uniquely if the order in which the elements are placed is preserved.

(3) The set G contains an *identity or unit element e* such that

$$eg = ge = g \text{ for any element } g \in G. \quad (3.2.3.9)$$

(4) For any element $g \in G$ there exists an *inverse element g^{-1}* such that

$$gg^{-1} = g^{-1}g = e. \quad (3.2.3.10)$$

The number of elements of a group G is called the *order of the group*. If the order of the group is finite, it is denoted by $|G|$.

The multiplication of group elements is, in general, not commutative, i.e. $g_i g_j \neq g_j g_i$ may hold for some $g_i, g_j \in G$. If the multiplication is commutative, i.e. if $g_i g_j = g_j g_i$ for all $g_i, g_j \in G$, then the group G is called a *commutative or Abelian group*. All groups of orders 1 to 5 are Abelian. In Abelian groups, an *additive notation* is sometimes used instead of the *multiplicative notation*, i.e. if g_i and g_k are elements of an Abelian group G then

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

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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

$$G = g_1F_1 \cup g_2F_1 \cup \dots \cup g_nF_1 = \bigcup_{i=1}^n g_iF_1, \quad (3.2.3.19)$$

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 $\{g_1, g_2, \dots, g_n\}$ 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

$$n = [G : F_1] = |G| : |F_1|, \quad (3.2.3.20)$$

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 ,

$$G = h_1L_1 \cup h_2L_1 \cup \dots \cup h_mL_1 = \bigcup_{j=1}^m h_jL_1, \quad (3.2.3.21)$$

where

$$m = [G : L_1] = |G| : |L_1|, \quad (3.2.3.22)$$

and the group L_1 into left cosets of F_1 ,

$$L_1 = p_1F_1 \cup p_2F_1 \cup \dots \cup p_dF_1 = \bigcup_{k=1}^d p_kF_1, \quad (3.2.3.23)$$

where

$$d = [L_1 : F_1] = |L_1| : |F_1|. \quad (3.2.3.24)$$

Then the decomposition of G into left cosets of F_1 can be written in the form

$$G = \bigcup_{j=1}^m \bigcup_{k=1}^d h_jp_kF_1 \quad (3.2.3.25)$$

and the index n of F_1 in G can be expressed as a product of indices m and d ,

$$n = [G : F_1] = [G : L_1][L_1 : F_1] = md. \quad (3.2.3.26)$$

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

$$gF_i g^{-1} = F_k, \quad g \in G. \quad (3.2.3.27)$$

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

$$gF_i g^{-1} = F_i, \quad g \in G, \quad (3.2.3.28)$$

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 ,

$$F_i \subseteq N_G(F_i) \subseteq G. \quad (3.2.3.29)$$

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 :

$$m = [G : N_G(F_i)] = |G| : |N_G(F_i)|, \quad (3.2.3.30)$$

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 ,

$$N_G(H) = G. \quad (3.2.3.31)$$

(3) Every element g of G commutes with H , or, equivalently, each left coset gH equals the right coset Hg :

$$gH = Hg \text{ for every } g \in G. \quad (3.2.3.32)$$

For a normal subgroup H of a group G a special symbol \triangleleft is often used instead of \subset , $H \triangleleft G$.

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3.2.3.2.7. Halving subgroups and dichromatic (black-and-white) groups

Any subgroup H of a group G of index 2, called a *halving subgroup*, is a normal subgroup. The decomposition of G into left cosets of H consists of two left cosets,

$$G = H \cup gH. \quad (3.2.3.33)$$

Sometimes it is convenient to distinguish elements of the coset gH from elements of the halving subgroup H . This can be achieved by attaching a sign (usually written as a superscript) to all elements of the coset. We shall use for this purpose the sign \blacklozenge . To aid understanding, we shall also mark for a while the elements of the group H with another sign, \heartsuit . The multiplication law for these ‘decorated elements’ can be written in the following form:

$$g_1 \heartsuit g_2 \heartsuit = g_3 \heartsuit, \quad g_4 \heartsuit g_5 \blacklozenge = g_6 \blacklozenge, \quad g_7 \blacklozenge g_8 \heartsuit = g_9 \heartsuit, \quad g_{10} \blacklozenge g_{11} \blacklozenge = g_{12} \heartsuit. \quad (3.2.3.34)$$

Now we replace the label \heartsuit by a dummy ‘no mark’ sign (*i.e.* we remove \heartsuit), but we still keep in mind the multiplication rules (3.2.3.34). Then the decomposition (3.2.3.33) becomes

$$G = H \cup g \blacklozenge H, \quad (3.2.3.33a)$$

since the coset $g \blacklozenge H$ assembles all marked elements and H consists of all bare elements of the group G .

The sign \blacklozenge can carry useful additional information, *e.g.* the application of labelled operations $g \blacklozenge$ is connected with some changes or new effects, whereas the application of a bare operation brings about no such changes or effects.

The label \blacklozenge can be replaced by various signs which can have different meanings. Thus in Chapter 3.3 a prime ‘ \prime ’ signifies a nontrivial twinning operation, in Chapter 1.5 it is associated with time inversion in magnetic structures, and in black-and-white patterns or structures a prime denotes an operation which exchanges black and white ‘colours’ (the qualifier ‘black-and-white’ concerns group operations, but not the black-and-white pattern itself). In Chapter 3.4, a star ‘ \ast ’ denotes a transposing operation which exchanges two domain states, while underlining signifies an operation exchanging two sides of an interface and underlined operations with a star signify twinning operations of a domain twin. Various interpretations of the label attached to the symbol of an operation have given rise to several designations of groups with partition (3.2.3.34): *black-and-white*, *dichromatic*, *magnetic*, *anti-symmetry*, *Shubnikov* or *Heech–Shubnikov* and other groups. For more details see Opechowski (1986).

3.2.3.2.8. Double cosets

Let F_1 and H_1 be two proper subgroups of the group G . The set of all distinct products $hg_j f$, where g_j is a fixed element of the group G and f and h run over all elements of the subgroups F_1 and H_1 , respectively, is called a *double coset of F_1 and H_1 in G* . The symbol of this double coset is $H_1 g_j F_1$,

$$F_1 g_j H_1 = \{fg_j h \mid \forall f \in F_1, \forall h \in H_1\}, \\ g_j \in G, F_1 \subset G, H_1 \subset G, \quad (3.2.3.35)$$

where the sign \forall means ‘for all’.

In the symmetry analysis of domain structures, only double cosets with $H_1 = F_1$ are used. We shall, therefore, formulate subsequent definitions and statements only for this special type of double coset.

The fixed element g_j is called the *representative of the double coset $F_1 g_j F_1$* . Any element of a double coset can be chosen as its representative.

Two double cosets are either identical or disjoint.

Proposition 3.2.3.6. The union of all distinct double cosets constitutes a partition of G and is called the *decomposition of the group G into double cosets of F_1* , since $F_1 F_1 = F_1$. If the set of double cosets of F_1 in G is finite, then the decomposition of G into the double cosets of F_1 can be written as

$$G = F_1 g_1 F_1 \cup F_1 g_2 F_1 \cup \dots \cup F_1 g_q F_1. \quad (3.2.3.36)$$

For the representative g_1 of the first double coset $F_1 g_1 F_1$ the unit element e is usually chosen, $g_1 = e$. Then the first double coset is identical with the subgroup F_1 .

A double coset $F_1 g_j F_1$ consists of left cosets of the form $f g_j F_1$, where $f \in F_1$. The number r of left cosets of F_1 in the double coset $F_1 g_j F_1$ is (Hall, 1959)

$$r = [F_1 : F_{1j}], \quad (3.2.3.37)$$

where

$$F_{1j} = F_1 \cap g_j F_1 g_j^{-1}. \quad (3.2.3.38)$$

The following definitions and statements are used in Chapter 3.4 for the double cosets $F_1 g_j F_1$ [for derivations and more details, see Janovec (1972)].

The inverse $(F_1 g_j F_1)^{-1}$ of a double coset $F_1 g_j F_1$ is a double coset $F_1 g_j^{-1} F_1$, which is either identical or disjoint with the double coset $F_1 g_j F_1$. The double coset that is its own inverse is called an *invertible (self-inverse, ambivalent) double coset*. The double coset that is disjoint with its inverse is called a *non-invertible (polar) double coset* and the double cosets $F_1 g_j F_1$ and $(F_1 g_j F_1)^{-1} = F_1 g_j^{-1} F_1$ are called *complementary polar double cosets*.

The inverse left coset $(g_j F_1)^{-1}$ contains representatives of all left cosets of the double coset $F_1 g_j^{-1} F_1$. If a left coset $g_j F_1$ belongs to an invertible double coset, then $(g_j F_1)^{-1}$ contains representatives of left cosets constituting the double coset $F_1 g_j F_1$. If a left coset $g_j F_1$ belongs to a non-invertible double coset, then $(g_j F_1)^{-1}$ contains representatives of left cosets constituting the complementary double coset $(F_1 g_j F_1)^{-1}$.

A double coset consisting of only one left coset,

$$F_1 g_j F_1 = g_j F_1, \quad (3.2.3.39)$$

is called a *simple double coset*. A double coset $F_1 g_j F_1$ is *simple* if and only if the inverse $(g_j F_1)^{-1}$ of the left coset $g_j F_1$ is again a left coset. For an invertible simple double coset $g_j F_1 = (g_j F_1)^{-1}$.

The union of all simple double cosets $F_1 g_j F_1 = g_j F_1$ in the double coset decomposition of G (3.2.3.36) constitutes the normalizer $N_G(F_1)$ (Speiser, 1927).

A double coset that comprises more than one left coset will be called a *multiple double coset*. Four types of double cosets FgF are displayed in Table 3.2.3.1. The double coset decompositions of all crystallographic point groups are available in the software *GI*KoBo-1* under *Subgroups\View\Twinning Group*.

Double cosets and the decomposition (3.2.3.36) of a group in double cosets are mathematical tools for partitioning a set of pairs of objects into equivalent classes (see Section 3.2.3.3.6). Such a division enables one to find possible twin laws and different types of domain walls that can appear in a domain structure resulting from a phase transition with a given symmetry descent (see Chapters 3.3 and 3.4).

More detailed introductions to group theory can be found in Budden (1972), Janssen (1973), Ledermann (1973), Rosen (1995), Shubnikov & Koptsik (1974), Vainshtein (1994) and Vainshtein *et*

Table 3.2.3.1. Four types of double cosets

	$FgF = gF$	$FgF \neq gF$
$FgF = (FgF)^{-1}$	Invertible simple	Invertible multiple
$FgF \cap (FgF)^{-1} = \emptyset$	Non-invertible simple	Non-invertible multiple

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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, \mathbf{A} a set of objects $\mathbf{S}_i, \mathbf{S}_j, \mathbf{S}_k, \dots$ and $\varphi : G \times \mathbf{A} \rightarrow \mathbf{A}$ a mapping that assigns to an ordered pair (g, \mathbf{S}_i) , where $g \in G, \mathbf{S}_i$ and \mathbf{S}_i are objects of the set \mathbf{A} :

$$\varphi : (g, \mathbf{S}_i) \mapsto \mathbf{S}_k, \quad g \in G, \quad \mathbf{S}_i, \mathbf{S}_k \in \mathbf{A}. \quad (3.2.3.46)$$

The ordered pair (g, \mathbf{S}_i) can often be written simply as a product $g\mathbf{S}_i$ and the mapping as an equation. Then the relation (3.2.3.46) can be expressed in a simpler form:

$$g\mathbf{S}_i = \mathbf{S}_k, \quad g \in G, \quad \mathbf{S}_i, \mathbf{S}_k \in \mathbf{A}. \quad (3.2.3.47)$$

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

$$e\mathbf{S}_i = \mathbf{S}_i \text{ for any } \mathbf{S}_i \in \mathbf{A}, \quad (3.2.3.48)$$

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

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

then the mapping φ is called an *action* (or *operation*) of a group G on a set \mathbf{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 $g\mathbf{S}_i = \mathbf{S}_k$ followed by the second action $h\mathbf{S}_k = \mathbf{S}_m$ gives the same result as if one first calculates the product $hg = p$ and then applies it to \mathbf{S}_i , $p\mathbf{S}_i = \mathbf{S}_m$.

When a group G , a set \mathbf{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* \mathbf{A} and the set \mathbf{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 $\mathbf{a}'_1, \mathbf{a}'_2, \mathbf{a}'_3$,

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

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

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

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

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 ,

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

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

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

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

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

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 ,

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

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:

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

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 $(\mathbf{S}_r, \mathbf{S}_s)$,

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

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

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

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

$$G = F_1 \cup F_1g_2F_1 \cup \dots \cup F_1g_jF_1 \cup \dots \cup F_1g_qF_1, \quad j = 1, 2, \dots, q. \tag{3.2.3.100}$$

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

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

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

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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