

3. PHASE TRANSITIONS, TWINNING AND DOMAIN STRUCTURES

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