

3.2. TWINNING AND DOMAIN STRUCTURES

al. (1995). More advanced books on group theory are, for example, Bradley & Cracknell (1972), Hall (1959), Lang (1965), Opechowski (1986), Robinson (1982) and Speiser (1927). Parts of group theory relevant to phase transitions and tensor properties are treated in the manual of the software *GI★KoBo-1*. Representations of the crystallographic groups are presented in Chapter 1.2 of this volume and in the software *GI★KoBo-1* (see the manual).

3.2.3.3. Action of a group on a set

3.2.3.3.1. Group action

A direct application of the set and group theory to our studies would hardly justify their presentation in the last two sections. However, an appropriate combination of these theories, called group action, forms a very useful tool for examining crystalline materials and domain structures in particular. In this section, the main concepts (action of a group on a set [a], orbits [o], stabilizers [s]) are explained and their application is illustrated with examples from crystallography, where the group G is either a crystallographic point group or space group (denoted \mathcal{G} , if necessary), and the set is the three-dimensional point space $E(3)$ [P], a crystal [C], a property tensor [T] and a subgroup of G [S]. Letters in square brackets in front of the sequential number of examples and definitions should aid navigation in the text.

Example [aP] 3.2.3.7. Crystals are objects in a three-dimensional space called point space. Points of this space form an infinite set which we denote $E(3)$. If one chooses a point O as the origin, then to each point $X \in E(3)$ one can assign the position vector $OX = \mathbf{r}$ of a vector space $V(3)$ [see, for example, *IT A* (2002), Part 8]. There is a one-to-one correspondence between points of the point space and corresponding position vectors of the vector space,

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

If one further selects three non-coplanar basic vectors $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$, then the position vector \mathbf{r} can be written as

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

where x_1, x_2, x_3 are coordinates of the point X .

Let G be a point group. An operation (isometry) $g \in G$ transforms (moves) the point X to a point X' with the position vector

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

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

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

where $D(g)_{ij}$ are components of a 3×3 matrix representing the operation g .

The described motion of the point X under the operation g can be formally expressed as a simple relation

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

the exact meaning of which can be formulated in terms introduced in Section 3.2.3.1 as a mapping φ that assigns to an ordered pair (g, X) a point X' of the set $E(3)$,

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

The mapping φ – *i.e.* a prescription for how to determine from g and X the resulting point X' – is defined by (3.2.3.40) to (3.2.3.43). The relation (3.2.3.44) should be considered as only a shorthand version of the explicit relation (3.2.3.45).

The action of a group on a set generalizes the described procedure to any group and any set. In this section, we shall use the term ‘object’ for an element of a set and the term ‘operation’ for an element of a group.

Definition [a] 3.2.3.8. Let G be a group, A a set of objects S_i, S_j, S_k, \dots and $\varphi : G \times A \rightarrow A$ a mapping that assigns to an ordered pair (g, S_i) , where $g \in G, S_i$ and S_i are objects of the set A :

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

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

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

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

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

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

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

then the mapping φ is called an *action* (or *operation*) of a group G on a set A , or just a *group action*.

We must note that the replacement of the explicit mapping (3.2.3.46) by a contracted version (3.2.3.47) is not always possible (see Example [aS] 3.2.3.11).

The condition (3.2.3.49) requires that the first action $gS_i = S_k$ followed by the second action $hS_k = S_m$ gives the same result as if one first calculates the product $hg = p$ and then applies it to S_i , $pS_i = S_m$.

When a group G , a set A , and a mapping φ fulfil the requirements (3.2.3.47) to (3.2.3.49), one says that G *acts* or *operates on* A and the set A is called a *G-set*.

Example [aC] 3.2.3.9. We shall examine the action of an isometry g on an ideal infinite crystal in the three-dimensional space. Let us choose four points (atoms) of the crystal that define three non-coplanar vectors $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ (*e.g.* basic lattice translations). These vectors will specify the *orientation of the crystal in space*. Let g be a point-group operation. This isometry g transforms (moves) points of the crystal to new positions and changes the orientation of the crystal to a new orientation specified by vectors $\mathbf{a}'_1, \mathbf{a}'_2, \mathbf{a}'_3$,

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

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