

3. PHASE TRANSITIONS, TWINNING AND DOMAIN STRUCTURES

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.* **A**, **B**, . . . , and capital bold letters, *e.g.* **S**, **M**, **N**, . . . or **S**<sub>1</sub>, **S**<sub>2</sub>, **S**<sub>3</sub>, . . . , 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*, . . . . 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 **S** belongs to the set **A**, one writes **S** ∈ **A**, in the opposite case **S** ∉ **A**. Sets consisting of a small number of elements can be expressed explicitly by writing their elements between curly braces, **A** = {**S**, **M**, **N**, **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* **A** consists of a finite number of elements and this number is denoted by |**A**|. An *infinite set* contains infinite number of elements and an *empty set*, denoted by ∅, contains no element. In what follows, the term ‘set’ will mean a ‘finite nonempty set’ unless explicitly stated otherwise.

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

The *intersection* of two sets **A** and **B**, **A** ∩ **B** or **B** ∩ **A**, is a set comprising all elements that belong both to **A** and to **B**. If the sets

**A** and **B** have no element in common, **A** ∩ **B** = ∅, then one says that the sets **A** and **B** are *disjoint*. The *union of sets* **A** and **B**, **A** ∪ **B** or **B** ∪ **A**, is a set consisting of all elements that belong either to **A** or to **B**. Sometimes the symbol + is used instead of the symbol ∪. The *difference of set A and B*, or the *complement of B in A*, **A** − **B**, comprises those elements of **A** that do not belong to **B**.

3.2.3.1.2. Pairs

A collection of two objects **S**<sub>*i*</sub> and **S**<sub>*k*</sub> 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 {**S**, **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 (**S**<sub>*i*</sub>, **S**<sub>*k*</sub>), consists of the *first* and the *second member* of the pair. If **S**<sub>*i*</sub> = **S**<sub>*k*</sub>, the ordered pair is called a *trivial ordered pair*, (**S**<sub>*i*</sub>, **S**<sub>*i*</sub>); if **S**<sub>*i*</sub> ≠ **S**<sub>*k*</sub> the pair (**S**<sub>*i*</sub>, **S**<sub>*k*</sub>) is a *non-trivial ordered pair*. The ordered pair (**S**<sub>*k*</sub>, **S**<sub>*i*</sub>) 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 **S**<sub>*i*</sub> and **S**<sub>*k*</sub> of an ordered pair (**S**<sub>*i*</sub>, **S**<sub>*k*</sub>) can either belong to one set, **S**<sub>*i*</sub> ∈ **A**, **S**<sub>*k*</sub> ∈ **A**, or each to a different set, **S**<sub>*i*</sub> ∈ **A**, **S**<sub>*k*</sub> ∈ **B**.

Two ordered pairs (**S**<sub>*i*</sub>, **S**<sub>*k*</sub>) and (**S**<sub>*m*</sub>, **S**<sub>*p*</sub>) are equal, (**S**<sub>*i*</sub>, **S**<sub>*k*</sub>) = (**S**<sub>*m*</sub>, **S**<sub>*p*</sub>), if and only if **S**<sub>*i*</sub> = **S**<sub>*m*</sub> and **S**<sub>*k*</sub> = **S**<sub>*p*</sub>.

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* **A** × **B** of two sets **A** and **B** is a set of *all* ordered pairs (**S**, **M**), where **S** ∈ **A**, **M** ∈ **B**. The sets **A** and **B** can be different or identical sets. If the sets **A** and **B** are finite, then the Cartesian product **A** × **B** consists of |**A**| · |**B**| ordered pairs.

3.2.3.1.3. Mappings

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

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