

## 8. INTRODUCTION TO SPACE-GROUP SYMMETRY

have to be augmented to  $[(n+1) \times 1]$  columns  $\mathbf{x}$  and  $\tilde{\mathbf{x}}$ . The motion is now described by the one matrix  $\mathbb{W}$  instead of the pair  $(\mathbf{W}, \mathbf{w})$ .

If the motion  $M$  is described by  $\mathbb{W}$ , the ‘inverse motion’  $M^{-1}$  is described by  $\mathbb{W}^{-1}$ , where  $(\mathbf{W}, \mathbf{w})^{-1} = (\mathbf{W}^{-1}, -\mathbf{W}^{-1}\mathbf{w})$ . Successive application of two motions,  $\mathbf{W}_1$  and  $\mathbf{W}_2$ , results in another motion  $\mathbf{W}_3$ :

$$\tilde{X} = \mathbf{W}_1 X \text{ and } \tilde{\tilde{X}} = \mathbf{W}_2 \tilde{X} = \mathbf{W}_2 \mathbf{W}_1 X = \mathbf{W}_3 X.$$

with  $\mathbf{W}_3 = \mathbf{W}_2 \mathbf{W}_1$ .

This can be described in matrix notation as follows

$$\tilde{\mathbf{x}} = \mathbf{W}_1 \mathbf{x} + \mathbf{w}_1$$

and

$$\tilde{\tilde{\mathbf{x}}} = \mathbf{W}_2 \tilde{\mathbf{x}} + \mathbf{w}_2 = \mathbf{W}_2 \mathbf{W}_1 \mathbf{x} + \mathbf{W}_2 \mathbf{w}_1 + \mathbf{w}_2 = \mathbf{W}_3 \mathbf{x} + \mathbf{w}_3,$$

with  $(\mathbf{W}_3, \mathbf{w}_3) = (\mathbf{W}_2 \mathbf{W}_1, \mathbf{W}_2 \mathbf{w}_1 + \mathbf{w}_2)$  or

$$\tilde{\tilde{\mathbf{x}}} = \mathbf{W}_1 \mathbf{x} \text{ and } \tilde{\tilde{\tilde{\mathbf{x}}}} = \mathbf{W}_2 \tilde{\tilde{\mathbf{x}}} = \mathbf{W}_2 \mathbf{W}_1 \mathbf{x} = \mathbf{W}_3 \mathbf{x}$$

with  $\mathbf{W}_3 = \mathbf{W}_2 \mathbf{W}_1$ .

It is a special advantage of the augmented matrices that successive application of motions is described by the product of the corresponding augmented matrices.

A point  $X$  is called a *fixed point* of the mapping  $M$  if it is invariant under the mapping, i.e.  $\tilde{X} = X$ .

In an  $n$ -dimensional Euclidean space  $E^n$ , three types of motions can be distinguished:

(1) *Translation*. In this case,  $\mathbf{W} = \mathbf{I}$ , where  $\mathbf{I}$  is the unit matrix; the vector  $\mathbf{w} = w_1 \mathbf{a}_1 + \dots + w_n \mathbf{a}_n$  is called the *translation vector*.

(2) *Motions with at least one fixed point*. In  $E^1$ ,  $E^2$  and  $E^3$ , such motions are called proper motions or *rotations* if  $\det(\mathbf{W}) = +1$  and improper motions if  $\det(\mathbf{W}) = -1$ . Improper motions are called *inversions* if  $\mathbf{W} = -\mathbf{I}$ ; *reflections* if  $\mathbf{W}^2 = \mathbf{I}$  and  $\mathbf{W} \neq -\mathbf{I}$ ; and *rotoinversions* in all other cases. The inversion is a rotation for spaces of even dimension, but an (improper) motion of its own kind in spaces of odd dimension. The origin is among the fixed points if  $\mathbf{w} = \mathbf{o}$ , where  $\mathbf{o}$  is the  $(n \times 1)$  column consisting entirely of zeros.

(3) *Fixed-point-free motions which are not translations*. In  $E^3$ , they are called *screw rotations* if  $\det(\mathbf{W}) = +1$  and *glide reflections* if  $\det(\mathbf{W}) = -1$ . In  $E^2$ , only glide reflections occur. No such motions occur in  $E^1$ .

In Fig. 8.1.2.2, the relations between the different types of motions in  $E^3$  are illustrated. The diagram contains all kinds of motions except the identity mapping  $I$  which leaves the whole space invariant and which is described by  $\mathbb{W} = I$ . Thus, it is simultaneously a special rotation (with rotation angle 0) and a special translation (with translation vector  $\mathbf{o}$ ).

So far, motions  $M$  in point space  $E^n$  have been considered. Motions give rise to mappings of the corresponding vector space  $\mathbf{V}^n$  onto itself. If  $M$  maps the points  $P_1$  and  $Q_1$  of  $E^n$  onto  $P_2$  and  $Q_2$ , the vector  $\overrightarrow{P_1 Q_1}$  is mapped onto the vector  $\overrightarrow{P_2 Q_2}$ . If the motion in  $E^n$  is described by  $\tilde{\mathbf{x}} = \mathbf{W}\mathbf{x} + \mathbf{w}$ , the vectors  $\mathbf{v}$  of  $\mathbf{V}^n$  are mapped according to  $\tilde{\mathbf{v}} = \mathbf{W}\mathbf{v}$ . In other words, of the linear and translation parts of the motion of  $E^n$ , only the linear part remains in the corresponding mapping of  $\mathbf{V}^n$  (*linear mapping*). This difference between the mappings in the two spaces is particularly obvious for translations. For a translation  $T$  with translation vector  $\mathbf{t} \neq \mathbf{o}$ , no fixed point exists in  $E^n$ , i.e. no point of  $E^n$  is mapped onto itself by  $T$ . In  $\mathbf{V}^n$ , however, any vector  $\mathbf{v}$  is mapped onto itself since the corresponding linear mapping is the identity mapping.

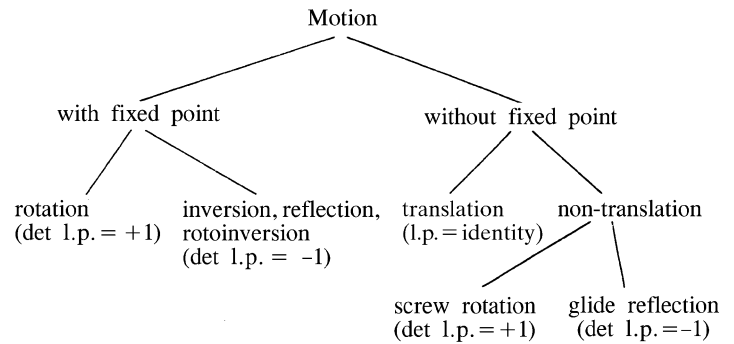


Fig. 8.1.2.2. Relations between the different kinds of motions in  $E^3$ ; det l.p. = determinant of the linear part. The identity mapping does not fit into this scheme properly and hence has been omitted.

## 8.1.3. Symmetry operations and symmetry groups

*Definition:* A *symmetry operation* of a given object in point space  $E^n$  is a motion of  $E^n$  which maps this object (point, set of points, crystal pattern etc.) onto itself.

*Remark:* Any motion may be a symmetry operation, because for any motion one can construct an object which is mapped onto itself by this motion.

For the set of *all* symmetry operations of a given object, the following relations hold:

(a) successive application of two symmetry operations of an object results in a third symmetry operation of that object;

(b) the inverse of a symmetry operation is also a symmetry operation;

(c) there exists an ‘identity operation’  $I$  which leaves each point of the space fixed:  $X \rightarrow X$ . This operation  $I$  is described (in any coordinate system) by  $(\mathbf{W}, \mathbf{w}) = (\mathbf{I}, \mathbf{o})$  or by  $\mathbb{W} = I$  and it is a symmetry operation of any object.

(d) The ‘associative law’  $(\mathbf{W}_3 \mathbf{W}_2) \mathbf{W}_1 = \mathbf{W}_3 (\mathbf{W}_2 \mathbf{W}_1)$  is valid. One can show, however, that in general the ‘commutative law’  $\mathbf{W}_2 \mathbf{W}_1 = \mathbf{W}_1 \mathbf{W}_2$  is not obeyed for symmetry operations.

The properties (a) to (d) are the group axioms. Thus, the set of all symmetry operations of an object forms a group, *the symmetry group of the object* or its *symmetry*. The mathematical theorems of *group theory*, therefore, may be applied to the symmetries of objects.

So far, only rather general objects have been considered. Crystallographers, however, are particularly interested in the symmetries of crystals. In order to introduce the concept of crystallographic symmetry operations, crystal structures, crystal patterns and lattices have to be taken into consideration. This will be done in the following section.

## 8.1.4. Crystal patterns, vector lattices and point lattices

Crystals are finite real objects in physical space which may be idealized by infinite three-dimensional periodic ‘crystal structures’ in point space. Three-dimensional periodicity means that there are translations among the symmetry operations of the object with the translation vectors spanning a three-dimensional space. Extending this concept of crystal structure to more general periodic objects and to  $n$ -dimensional space, one obtains the following definition:

*Definition:* An object in  $n$ -dimensional point space  $E^n$  is called an  $n$ -dimensional *crystallographic pattern* or, for short, *crystal pattern* if among its symmetry operations

(i) there are  $n$  translations, the translation vectors  $\mathbf{t}_1, \dots, \mathbf{t}_n$  of which are linearly independent,