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

If the motion M is described by $\mathbb{W}$, the 'inverse motion' M^{-1} is described by $\mathbb{W}^{-1}$, where $(\boldsymbol{W},\boldsymbol{w})^{-1} = (\boldsymbol{W}^{-1}, -\boldsymbol{W}^{-1}\boldsymbol{w})$. Successive application of two motions, W_1 and W_2, results in another motion W_3:

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

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

This can be described in matrix notation as follows

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

and

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

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

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

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

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, $\boldsymbol{W} = \boldsymbol{I}$, where $\boldsymbol{I}$ is the unit matrix; the vector $\mathbf{w} = w_1\mathbf{a}_1 + \ldots + w_n\mathbf{a}_n$ 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 $\det(\boldsymbol{W}) = +1$ and improper motions if $\det(\boldsymbol{W}) = -1$. Improper motions are called *inversions* if $\boldsymbol{W} = -\boldsymbol{I}$; *reflections* if $\boldsymbol{W}^2 = \boldsymbol{I}$ and $\boldsymbol{W} \neq -\boldsymbol{I}$; 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 $\boldsymbol{w} = \boldsymbol{o}$, where $\boldsymbol{o}$ 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 $\det(\boldsymbol{W}) = +1$ and *glide reflections* if $\det(\boldsymbol{W}) = -1$. 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 $\mathbb{W} = \mathbb{I}$. Thus, it is simultaneously a special rotation (with rotation angle 0) and a special translation (with translation vector $\mathbf{0}$).

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 $\overrightarrow{P_1Q_1}$ is mapped onto the vector $\overrightarrow{P_2Q_2}$. If the motion in E^n is described by $\tilde{\boldsymbol{x}} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{w}$, the vectors $\mathbf{v}$ of $\mathbf{V}^n$ are mapped according to $\tilde{\mathbf{v}} = \boldsymbol{W}\mathbf{v}$. 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 $\mathbf{t} \neq \mathbf{0}$, 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.

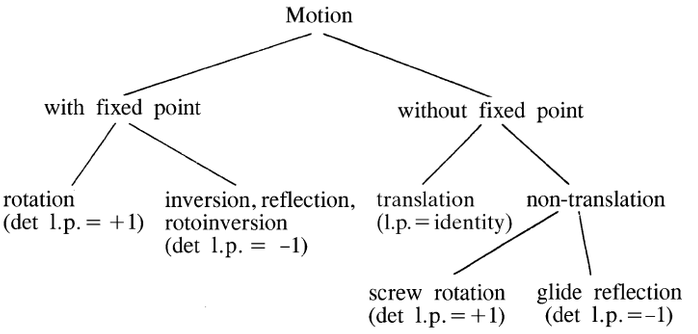

Fig. 8.1.2.2. Relations between the different kinds of motions in E^3; det l.p. = determinant of the linear part. The identity mapping does not fit into this scheme properly and hence has been omitted.

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 $(\boldsymbol{W},\boldsymbol{w}) = (\boldsymbol{I},\boldsymbol{o})$ or by $\mathbb{W} = \mathbb{I}$ and it is a symmetry operation of any object.

(*d*) The 'associative law' $(\mathsf{W}_3\mathsf{W}_2)\mathsf{W}_1 = \mathsf{W}_3(\mathsf{W}_2\mathsf{W}_1)$ is valid.

One can show, however, that in general the 'commutative law' $\mathsf{W}_2\mathsf{W}_1 = \mathsf{W}_1\mathsf{W}_2$ 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 $\mathbf{t}_1, \ldots, \mathbf{t}_n$ of which are linearly independent,

(ii) all translation vectors, except the zero vector **o**, have a length of at least $d > 0$.

Condition (i) guarantees the n-dimensional periodicity and thus excludes subperiodic symmetries like layer groups, rod groups and frieze groups. Condition (ii) takes into account the finite size of atoms in actual crystals.

Successive application of two translations of a crystal pattern results in another translation, the translation vector of which is the (vector) sum of the original translation vectors. Consequently, in addition to the n linearly independent translation vectors $\mathbf{t}_1, \ldots, \mathbf{t}_n$, all (infinitely many) vectors $\mathbf{t} = u_1\mathbf{t}_1 + \ldots + u_n\mathbf{t}_n$ ($u_1, \ldots, u_n$ arbitrary integers) are translation vectors of the pattern. Thus, infinitely many translations belong to each crystal pattern. The periodicity of crystal patterns is represented by their lattices. It is useful to distinguish two kinds of lattices: vector lattices and point lattices. This distinction corresponds to that between vector space and point space, discussed above. The vector lattice is treated first.

Definition: The (infinite) set of *all* translation vectors of a crystal pattern is called the lattice of translation vectors or the *vector lattice* **L** of this crystal pattern.

In principle, any set of n linearly independent vectors may be used as a basis of the vector space $\mathbf{V}^n$. Most of these sets, however, result in a rather complicated description of a given vector lattice. The following theorem shows that among the (infinitely many) possible bases of the vector space $\mathbf{V}^n$ special bases always exist, referred to which the survey of a given vector lattice becomes particularly simple.

Definitions: (1) A basis of n vectors $\mathbf{a}_1, \ldots, \mathbf{a}_n$ of $\mathbf{V}^n$ is called a *crystallographic basis* of the n-dimensional vector lattice **L** if *every* integral linear combination $\mathbf{t} = u_1\mathbf{a}_1 + \ldots + u_n\mathbf{a}_n$ is a lattice vector of **L**. (2) A basis is called a primitive crystallographic basis of **L** or, for short, a *primitive basis* if it is a crystallographic basis and if, furthermore, *every* lattice vector **t** of **L** may be obtained as an *integral* linear combination of the basis vectors.

The distinction between these two kinds of bases can be expressed as follows. Referred to a crystallographic basis, the coefficients of each lattice vector must be either integral or rational. Referred to a primitive crystallographic basis, only integral coefficients occur. It should be noted that nonprimitive crystallographic bases are used conventionally for the description of 'centred lattices', whereas reduced bases are always primitive; see Chapter 9.2.

Example

The basis used conventionally for the description of the 'cubic body-centred lattice' is a crystallographic basis because the basis vectors **a**, **b**, **c** are lattice vectors. It is not a primitive basis because lattice vectors with non-integral but rational coefficients exist, *e.g.* the vector $\frac{1}{2}\mathbf{a} + \frac{1}{2}\mathbf{b} + \frac{1}{2}\mathbf{c}$. The bases $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b} + \mathbf{c})$, $\mathbf{b}' = \frac{1}{2}(\mathbf{a} - \mathbf{b} + \mathbf{c})$, $\mathbf{c}' = \frac{1}{2}(\mathbf{a} + \mathbf{b} - \mathbf{c})$ or $\mathbf{a}'' = \mathbf{a}$, $\mathbf{b}'' = \mathbf{b}$, $\mathbf{c}'' = \frac{1}{2}(\mathbf{a} + \mathbf{b} + \mathbf{c})$ are primitive bases. In the first of these bases, the vector $\frac{1}{2}(\mathbf{a} + \mathbf{b} + \mathbf{c})$ is given by $\mathbf{a}' + \mathbf{b}' + \mathbf{c}'$, in the second basis by $\mathbf{c}''$, both with integral coefficients only.

Fundamental theorem on vector lattices: For every vector lattice **L** primitive bases exist.

It can be shown that (in dimensions $n > 1$) the number of primitive bases for each vector lattice is infinite. There exists, however, a procedure called 'basis reduction' (*cf.* Chapter 9.2), which uniquely selects one primitive basis from this infinite set, thus permitting unambiguous description and comparison of vector lattices. Although such a reduced primitive basis always *can* be selected, in many cases conventional coordinate systems are chosen with nonprimitive rather than primitive crystallographic bases. The reasons are given in Section 8.3.1. The term 'primitive' is used not only for bases of lattices but also with respect to the lattices themselves, as in the crystallographic literature a *vector lattice* is frequently called *primitive* if its *conventional basis is primitive.*

With the help of the vector lattices defined above, the concept of point lattices will be introduced.

Definition: Given an arbitrary point X_0 in point space and a vector lattice **L** consisting of vectors $\mathbf{t}_j$, the set of all points X_j with $\overrightarrow{X_0X_j} = \mathbf{t}_j$ is called the *point lattice* belonging to X_0 and **L**.

A point lattice can be visualized as the set of end-points of all vectors of **L**, where **L** is attached to an arbitrary point X_0 of point space. Because each point X of point space could be chosen as the point X_0, an infinite set of point lattices belongs to each vector lattice. Frequently, the point X_0 is chosen as the origin of the coordinate system of the point space.

An important aspect of a lattice is its *unit cell*.

Definition: If $\mathbf{a}_1, \ldots, \mathbf{a}_n$ is a crystallographic basis of a vector lattice **L**, the set of all vectors $x_1\mathbf{a}_1 + \ldots + x_n\mathbf{a}_n$ with $0 \leq x_i < 1$ is called a *unit cell of the vector lattice.*

The concept of a 'unit cell' is not only applied to vector lattices in vector space but also more often to crystal structures or crystal patterns in point space. Here the coordinate system $(O, \mathbf{a}_1, \ldots, \mathbf{a}_n)$ and the origin X_0 of the unit cell have to be chosen. In most cases $X_0 = O$ is taken, but in general we have the following definition:

Definition: Given a crystallographic coordinate system $(O, \mathbf{a}_1, \ldots, \mathbf{a}_n)$ of a crystal pattern and a point X_0 with coordinates x_{0i}, a *unit cell of the crystal pattern* is the set of all points X with coordinates x_i such that the equation $0 \leq x_i - x_{0i} < 1$ $(i = 1, \ldots, n)$ holds.

Obviously, the term 'unit cell' may be transferred to real crystals. As the volume of the unit cell and the volumes of atoms are both finite, only a *finite* number N of atoms can occur in a unit cell of a crystal. A crystal structure, therefore, may be described in two ways:

(*a*) One starts with an arbitrary unit cell and builds up the whole crystal structure by infinite repetition of this unit cell. The crystal structure thus consists of an infinite number of finite 'building blocks', each building block being a unit cell.

(*b*) One starts with a point X_1 representing the centre of an atom. To this point belong an infinite number of translationally equivalent points X_j, *i.e.* points for which the vectors $\overrightarrow{X_1X_j}$ are lattice vectors. In this way, from each of the points X_i $(i = 1, \ldots, N)$ within the unit cell a point lattice of translationally equivalent points is obtained. The crystal structure is then described by a finite number of interpenetrating infinite point lattices.

In most cases, one is not interested in the orientation of the vector lattice or the point lattices of a crystal structure in space, but only in the shape and size of a unit cell. From this point of view, a three-dimensional lattice is fully described by the lengths a, b and c of the basis vectors **a**, **b** and **c** and by the three interaxial angles α, β and γ. These data are called the *lattice parameters*, *cell parameters* or *lattice constants* of both the vector lattice and the associated point lattices of the crystal structure.

8.1.5. Crystallographic symmetry operations

Crystallographic symmetry operations are special motions.

Definition: A motion is called a *crystallographic symmetry operation* if a crystal pattern exists for which it is a symmetry operation.