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1.5. Crystallographic viewpoints in the classification of space-group representations

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1.5.1. List of symbols

$\mathcal{G}$; $\mathcal{S}$	Group, especially space group; site-symmetry group
G	Element of group $\mathcal{G}$
$\mathcal{G}_0$	Symmorphic space group
$\mathcal{P}$ or $\bar{\mathcal{G}}$	Point group of space group $\mathcal{G}$
$\mathcal{T}$	Translation subgroup of space group $\mathcal{G}$
$\boldsymbol{R}, \boldsymbol{S}$; $\boldsymbol{W}$	Matrix; matrix part of a symmetry operation
$\boldsymbol{w}$	Column part of a symmetry operation
X	Point of point space
x, y, z; x_i	Coordinates of a point or coefficients of a vector
$\boldsymbol{x}$	Column of point coordinates or of vector coefficients
L	Vector lattice of the space group $\mathcal{G}$
$\mathbf{a}, \mathbf{b}, \mathbf{c}$ or $(\mathbf{a}_k)^T$	Basis vectors or row of basis vectors of the lattice **L** of $\mathcal{G}$
t	Vector of the lattice **L** of $\mathcal{G}$
$\mathbf{L}^*$	Reciprocal lattice of the space group $\mathcal{G}$
$\mathbf{a}^*, \mathbf{b}^*, \mathbf{c}^*$ or $(\mathbf{a}_k^*)$	Basis vectors or column of basis vectors of the reciprocal lattice $\mathbf{L}^*$
K	Vector of the reciprocal lattice $\mathbf{L}^*$
k	Vector of reciprocal space
$\mathcal{G}^*$	Reciprocal-space group
$\bar{\mathcal{G}}^{\mathbf{k}}$	Little co-group of **k**
$\mathcal{L}^{\mathbf{k}}$	Little group of **k**
$\Gamma(\mathcal{G})$	(Matrix) representation of $\mathcal{G}$

1.5.2. Introduction

This new chapter on representations widens the scope of the general topics of reciprocal space treated in this volume.

Space-group representations play a growing role in physical applications of crystal symmetry. They are treated in a number of papers and books but comparison of the terms and the listed data is difficult. The main reason for this is the lack of standards in the classification and nomenclature of representations. As a result, the reader is confronted with different numbers of types and barely comparable notations used by the different authors, see *e.g.* Stokes & Hatch (1988), Table 7.

The **k** vectors, which can be described as vectors in reciprocal space, play a decisive role in the description and classification of space-group representations. Their symmetry properties are determined by the so-called *reciprocal-space group* $\mathcal{G}^*$ which is always isomorphic to a symmorphic space group $\mathcal{G}_0$. The different symmetry types of **k** vectors correspond to the different kinds of point orbits in the symmorphic space groups $\mathcal{G}_0$. The classification of point orbits into Wyckoff positions in *International Tables for Crystallography* Volume A (*IT* A) (1995) can be used directly to classify the irreducible representations of a space group, abbreviated *irreps*; the Wyckoff positions of the symmorphic space groups $\mathcal{G}_0$ form a basis for a *natural* classification of the irreps. This was first discovered by Wintgen (1941). Similar results have been obtained independently by Raghavacharyulu (1961), who introduced the term reciprocal-space group. In this chapter a classification of irreps is provided which is based on Wintgen's idea.

Although this idea is now more than 50 years old, it has been utilized only rarely and has not yet found proper recognition in the literature and in the existing tables of space-group irreps. Slater (1962) described the correspondence between the special **k** vectors of the Brillouin zone and the Wyckoff positions of space group $Pm\bar{3}m$. Similarly, Jan (1972) compared Wyckoff positions with points of the Brillouin zone when describing the symmetry $Pm\bar{3}$ of the Fermi surface for the pyrite structure. However, the widespread tables of Miller & Love (1967), Zak *et al.* (1969), Bradley & Cracknell (1972) (abbreviated as BC), Cracknell *et al.* (1979) (abbreviated as CDML), and Kovalev (1986) have not made use of this kind of classification and its possibilities, and the existing tables are unnecessarily complicated, *cf.* Boyle (1986).

In addition, historical reasons have obscured the classification of irreps and impeded their application. The first considerations of irreps dealt only with space groups of translation lattices (Bouckaert *et al.*, 1936). Later, other space groups were taken into consideration as well. Instead of treating these (lower) symmetries as such, their irreps were derived and classified by starting from the irreps of lattice space groups and proceeding to those of lower symmetry. This procedure has two consequences:

(1) those **k** vectors that are special in a lattice space group are also correspondingly listed in the low-symmetry space group even if they have lost their special properties due to the symmetry reduction;

(2) during the symmetry reduction unnecessary new types of **k** vectors and symbols for them are introduced.

The use of the reciprocal-space group $\mathcal{G}^*$ avoids both these detours.

In this chapter we consider in more detail the reciprocal-space-group approach and show that widely used crystallographic conventions can be adopted for the classification of space-group representations. Some basic concepts are developed in Section 1.5.3. Possible conventions are discussed in Section 1.5.4. The consequences and advantages of this approach are demonstrated and discussed using examples in Section 1.5.5.

1.5.3. Basic concepts

The aim of this section is to give a brief overview of some of the basic concepts related to groups and their representations. Its content should be of some help to readers who wish to refresh their knowledge of space groups and representations, and to familiarize themselves with the kind of description in this chapter. However, it can not serve as an introductory text for these subjects. The interested reader is referred to books dealing with space-group theory, representations of space groups and their applications in solid-state physics: see Bradley & Cracknell (1972) or the forthcoming Chapter 1.2 of *IT* D (*Physical properties of crystals*) by Janssen (2001).

1.5.3.1. *Representations of finite groups*

Group theory is the proper tool for studying symmetry in science. The elements of the crystallographic groups are rigid motions (isometries) with regard to performing one after another. The set of all isometries that map an object onto itself always fulfils the group postulates and is called the symmetry or the symmetry group of that object; the isometry itself is called a symmetry operation. Symmetry groups of crystals are dealt with in this chapter. In addition, groups of matrices with regard to matrix multiplication (matrix groups) are considered frequently. Such groups will sometimes be called realizations or representations of abstract groups.

Many applications of group theory to physical problems are closely related to representation theory, *cf.* Rosen (1981) and

references therein. In this section, matrix representations Γ of finite groups $\mathcal{G}$ are considered. The concepts of *homomorphism* and *matrix groups* are of essential importance.

A group $\mathcal{B}$ is a homomorphic image of a group $\mathcal{A}$ if there exists a mapping of the elements A_i of $\mathcal{A}$ onto the elements B_k of $\mathcal{B}$ that preserves the multiplication relation (in general several elements of $\mathcal{A}$ are mapped onto one element of $\mathcal{B}$): if $\mathsf{A}_i \rightarrow \mathsf{B}_i$ and $\mathsf{A}_k \rightarrow \mathsf{B}_k$, then $\mathsf{A}_i\mathsf{A}_k \rightarrow \mathsf{B}_i\mathsf{B}_k$ holds for all elements of $\mathcal{A}$ and $\mathcal{B}$ (the image of the product is equal to the product of the images). In the special case of a one-to-one mapping, the homomorphism is called an *isomorphism*.

A matrix group is a group whose elements are non-singular square matrices. The law of combination is matrix multiplication and the group inverse is the inverse matrix. In the following we will be concerned with some basic properties of finite matrix groups relevant to representations.

Let $\mathcal{M}_1$ and $\mathcal{M}_2$ be two matrix groups whose matrices are of the same dimension. They are said to be equivalent if there exists a (non-singular) matrix $\boldsymbol{S}$ such that $\mathcal{M}_2 = \boldsymbol{S}^{-1}\mathcal{M}_1\boldsymbol{S}$ holds. Equivalence implies isomorphism but the inverse is not true: two matrix groups may be isomorphic without being equivalent. According to the theorem of Schur-Auerbach, every finite matrix group is equivalent to a unitary matrix group (by a unitary matrix group we understand a matrix group consisting entirely of unitary matrices).

A matrix group $\mathcal{M}$ is *reducible* if it is equivalent to a matrix group in which every matrix $\boldsymbol{M}$ is of the form

$$\boldsymbol{R} = \begin{pmatrix} \boldsymbol{D}_1 & \boldsymbol{X} \\ \boldsymbol{O} & \boldsymbol{D}_2 \end{pmatrix},$$

see *e.g.* Lomont (1959), p. 47. The group $\mathcal{M}$ is *completely reducible* if it is equivalent to a matrix group in which for all matrices $\boldsymbol{R}$ the submatrices $\boldsymbol{X}$ are $\boldsymbol{O}$ matrices (consisting of zeros only). According to the theorem of Maschke, a finite matrix group is completely reducible if it is reducible. A matrix group is *irreducible* if it is not reducible.

A (matrix) representation $\Gamma(\mathcal{G})$ of a group $\mathcal{G}$ is a homomorphic mapping of $\mathcal{G}$ onto a matrix group $\mathcal{M}(\mathcal{G})$. In a representation Γ every element $\mathsf{G} \in \mathcal{G}$ is associated with a matrix $\boldsymbol{M}(\mathsf{G})$. The dimension of the matrices is called the dimension of the representation.

The above-mentioned theorems on finite matrix groups can be applied directly to representations: we can restrict the considerations to unitary representations only. Further, since every finite matrix group is either completely reducible into irreducible constituents or irreducible, it follows that the infinite set of all matrix representations of a group is known in principle once the irreducible representations are known. Naturally, the question of how to construct all nonequivalent irreducible representations of a finite group and how to classify them arises.

Linear representations are especially important for applications. In this chapter only linear representations of space groups will be considered. Realizations and representations are homomorphic images of abstract groups, but not all of them are linear. In particular, the action of space groups on point space is a nonlinear realization of the abstract space groups because isometries and thus symmetry operations W of space groups $\mathcal{G}$ are nonlinear operations. The same holds for their description by matrix-column pairs $(\boldsymbol{W}, \boldsymbol{w})$,† by the general position, or by augmented (4×4) matrices, see *IT* A, Part 8. Therefore, the isomorphic matrix representation of a space group, mostly used by crystallographers and listed in the space-group tables of *IT* A as the general position, is not linear.

† In physics often written as the Seitz symbol $(\boldsymbol{W}|\boldsymbol{w})$.

1.5.3.2. *Space groups*

In crystallography one deals with real crystals. In many cases the treatment of the crystal is much simpler, but nevertheless describes the crystal and its properties very well, if the real crystal is replaced by an 'ideal crystal'. The real crystal is then considered to be a finite piece of an undisturbed, periodic, and thus infinitely extended arrangement of particles or their centres: ideal crystals are periodic objects in three-dimensional point space E^3, also called direct space. Periodicity means that there are translations among the symmetry operations of ideal crystals. The symmetry group of an ideal crystal is called its space group $\mathcal{G}$.

Space groups $\mathcal{G}$ are of special interest for our problem because:

(1) their irreps are the subject of the classification to be discussed;

(2) this classification makes use of the isomorphism of certain groups to the so-called symmorphic space groups $\mathcal{G}_0$.

Therefore, space groups are introduced here in a slightly more detailed manner than the other concepts. In doing this we follow the definitions and symbolism of *IT* A, Part 8.

To each space group $\mathcal{G}$ belongs an infinite set $\mathcal{T}$ of translations, the *translation lattice* of $\mathcal{G}$. The lattice $\mathcal{T}$ forms an infinite Abelian invariant subgroup of $\mathcal{G}$. For each translation its translation vector is defined. The set of all translation vectors is called the *vector lattice* $\mathbf{L}$ of $\mathcal{G}$. Because of the finite size of the atoms constituting the real crystal, the lengths of the translation vectors of the ideal crystal cannot be arbitrarily small; rather there is a lower limit $\delta > 0$ for their length in the range of a few Å.

When referred to a coordinate system $(O, \mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3)$, consisting of an origin O and a basis $\mathbf{a}_k$, the elements W, *i.e.* the symmetry operations of the space group $\mathcal{G}$, are described by matrix-column pairs $(\boldsymbol{W}, \boldsymbol{w})$ with matrix part $\boldsymbol{W}$ and column part $\boldsymbol{w}$. The translations of $\mathcal{G}$ are represented by pairs $(\boldsymbol{I}, \boldsymbol{t}_i)$, where $\boldsymbol{I}$ is the (3×3) unit matrix and $\boldsymbol{t}_i$ is the column of coefficients of the translation vector $\mathbf{t}_i \in \mathbf{L}$. The basis can always be chosen such that all columns $\boldsymbol{t}_i$ and no other columns of translations consist of integers. Such a basis $\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3$ is called a *primitive basis*. For each vector lattice $\mathbf{L}$ there exists an infinite number of primitive bases.

The space group $\mathcal{G}$ can be decomposed into left cosets relative to $\mathcal{T}$:

$$\mathcal{G} = \mathcal{T} \cup (\boldsymbol{W}_2, \boldsymbol{w}_2)\mathcal{T} \cup \ldots \cup (\boldsymbol{W}_i, \boldsymbol{w}_i)\mathcal{T} \cup \ldots \cup (\boldsymbol{W}_n, \boldsymbol{w}_n)\mathcal{T}. \quad (1.5.3.1)$$

The coset representatives form the finite set $\mathrm{V} = \{(\boldsymbol{W}_v, \boldsymbol{w}_v)\}, v = 1, \ldots, n$, with $(\boldsymbol{W}_1, \boldsymbol{w}_1) = (\boldsymbol{I}, \boldsymbol{o})$, where $\boldsymbol{o}$ is the column consisting of zeros only. The factor group $\mathcal{G}/\mathcal{T}$ is isomorphic to the *point group* $\mathcal{P}$ of $\mathcal{G}$ (called $\bar{\mathcal{G}}$ in books on representation theory) describing the symmetry of the external shape of the macroscopic crystal and being represented by the matrices $\boldsymbol{W}_1, \boldsymbol{W}_2, \ldots, \boldsymbol{W}_n$. If V can be chosen such that all $\boldsymbol{w}_v = \boldsymbol{o}$, then $\mathcal{G}$ is called a *symmorphic space group* $\mathcal{G}_0$. A symmorphic space group can be recognized easily from its conventional Hermann–Mauguin symbol which does not contain any screw or glide component. In terms of group theory, a symmorphic space group is the semidirect product of $\mathcal{T}$ and $\mathcal{P}$, *cf.* BC, p. 44. In symmorphic space groups $\mathcal{G}_0$ (and in no others) there are site-symmetry groups which are isomorphic to the point group $\mathcal{P}$ of $\mathcal{G}_0$.

Space groups can be classified into 219 (*affine*) *space-group types* either by isomorphism or by affine equivalence; the 230 *crystallographic* space-group types are obtained by restricting the transformations available for affine equivalence to those with positive determinant, *cf. IT* A, Section 8.2.1. Many important properties of space groups are shared by all space groups of a type. In such a case one speaks of *properties of the type*. For example, if a space group is symmorphic, then all space groups of its type are

symmorphic, so that one normally speaks of a symmorphic space-group type.

With the concept of symmorphic space groups one can also define the arithmetic crystal classes: Let $\mathcal{G}_0$ be a symmorphic space group referred to a primitive basis and $\mathrm{V} = \{(\boldsymbol{W}_v, \boldsymbol{w}_v)\}$ its set of coset representatives with $\boldsymbol{w}_v = \boldsymbol{o}$ for all columns. To $\mathcal{G}_0$ all those space groups $\mathcal{G}$ can be assigned for which a primitive basis can be found such that the matrix parts $\boldsymbol{W}_v$ of their sets V are the same as those of $\mathcal{G}_0$, only the columns $\boldsymbol{w}_v$ may differ. In this way, to a type of symmorphic space groups $\mathcal{G}_0$, other types of space groups are assigned, *i.e.* the space-group types are classified according to the symmorphic space-group types. These classes are called *arithmetic crystal classes* of space groups or of space-group types.

There are 73 arithmetic crystal classes corresponding to the 73 types of symmorphic space groups; between 1 and 16 space-group types belong to an arithmetic crystal class. A matrix-algebraic definition of arithmetic crystal classes and a proposal for their nomenclature can be found in *IT* A, Section 8.2.2; see also Section 8.3.4 and Table 8.2.

1.5.3.3. *Representations of the translation group $\mathcal{T}$ and the reciprocal lattice*

For representation theory we follow the terminology of BC and CDML.

Let $\mathcal{G}$ be referred to a primitive basis. For the following, the infinite set of translations, based on discrete cyclic groups of infinite order, will be replaced by a (very large) finite set in the usual way. One assumes the Born–von Karman boundary conditions

$$(\boldsymbol{I}, \boldsymbol{t}_{bi})^{N_i} = (\boldsymbol{I}, N_i) = (\boldsymbol{I}, \boldsymbol{o}) \qquad (1.5.3.2)$$

to hold, where $\boldsymbol{t}_{bi} = (1,0,0)$, (0, 1, 0) or (0, 0, 1) and N_i is a large integer for $i = 1$, 2 or 3, respectively. Then for any lattice translation $(\boldsymbol{I}, \boldsymbol{t})$,

$$(\boldsymbol{I}, \boldsymbol{Nt}) = (\boldsymbol{I}, \boldsymbol{o}) \qquad (1.5.3.3)$$

holds, where $\boldsymbol{Nt}$ is the column $(N_1 t_1, N_2 t_2, N_3 t_3)$. If the (infinitely many) translations mapped in this way onto $(\boldsymbol{I}, \boldsymbol{o})$ form a normal subgroup $\mathcal{T}_1$ of $\mathcal{G}$, then the mapping described by (1.5.3.3) is a homomorphism. There exists a factor group $\mathcal{G}' = \mathcal{G}/\mathcal{T}_1$ of $\mathcal{G}$ relative to $\mathcal{T}_1$ with translation subgroup $\mathcal{T}' = \mathcal{T}/\mathcal{T}_1$ which is finite and is sometimes called the *finite space group*.

Only the irreducible representations (irreps) of these finite space groups will be considered. The definitions of space-group type, symmorphic space group *etc.* can be transferred to these groups. Because $\mathcal{T}$ is Abelian, $\mathcal{T}'$ is also Abelian. Replacing the space group $\mathcal{G}$ by $\mathcal{G}'$ means that the especially well developed theory of representations of finite groups can be applied, *cf.* Lomont (1959), Jansen & Boon (1967). For convenience, the prime $'$ will be omitted and the symbol $\mathcal{G}$ will be used instead of $\mathcal{G}'$; $\mathcal{T}'$ will be denoted by $\mathcal{T}$ in the following.

Because $\mathcal{T}$ (formerly $\mathcal{T}'$) is Abelian, its irreps $\Gamma(\mathcal{T})$ are one-dimensional and consist of (complex) roots of unity. Owing to equations (1.5.3.2) and (1.5.3.3), the irreps $\Gamma^{q_1 q_2 q_3}[(\boldsymbol{I}, \boldsymbol{t})]$ of $\mathcal{T}$ have the form

$$\Gamma^{q_1 q_2 q_3}[(\boldsymbol{I}, \boldsymbol{t})] = \exp\left[-2\pi i\left(q_1 \frac{t_1}{N_1} + q_2 \frac{t_2}{N_2} + q_3 \frac{t_3}{N_3}\right)\right], \quad (1.5.3.4)$$

where $\boldsymbol{t}$ is the column (t_1, t_2, t_3), $q_j = 0, 1, 2, \ldots, N_j - 1, j = 1, 2, 3$, and t_k and q_j are integers.

Given a primitive basis $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ of $\mathbf{L}$, mathematicians and crystallographers define the *basis of the dual or reciprocal lattice* $\mathbf{L}^*$ by

$$\mathbf{a}_i \cdot \mathbf{a}_j^* = \delta_{ij}, \qquad (1.5.3.5)$$

where $\mathbf{a} \cdot \mathbf{a}^*$ is the scalar product between the vectors and δ_{ij} is the unit matrix (see *e.g.* Chapter 1.1, Section 1.1.3). Texts on the physics of solids redefine the basis $\mathbf{a}_1^*, \mathbf{a}_2^*, \mathbf{a}_3^*$ of the *reciprocal lattice* $\mathbf{L}^*$, lengthening each of the basis vectors $\mathbf{a}_j^*$ by the factor 2π. Therefore, in the physicist's convention the relation between the bases of direct and reciprocal lattice reads (*cf.* BC, p. 86):

$$\mathbf{a}_i \cdot \mathbf{a}_j^* = 2\pi\delta_{ij}. \qquad (1.5.3.6)$$

In the present chapter only the physicist's basis of the reciprocal lattice is employed, and hence the use of $\mathbf{a}_j^*$ should not lead to misunderstandings. The set of all vectors $\mathbf{K}$,†

$$\mathbf{K} = k_1\mathbf{a}_1^* + k_2\mathbf{a}_2^* + k_3\mathbf{a}_3^*, \qquad (1.5.3.7)$$

k_i integer, is called the lattice reciprocal to $\mathbf{L}$ or the *reciprocal lattice* $\mathbf{L}^*$.‡

If one adopts the notation of *IT* A, Part 5, the basis of direct space is denoted by a row $(\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3)^T$, where $(\ )^T$ means transposed. For reciprocal space, the basis is described by a column $(\mathbf{a}_1^*, \mathbf{a}_2^*, \mathbf{a}_3^*)$.

To each lattice generated from a basis $(\mathbf{a}_i)^T$ a reciprocal lattice is generated from the basis $(\mathbf{a}_j^*)$. Both lattices, $\mathbf{L}$ and $\mathbf{L}^*$, can be compared most easily by referring the direct lattice $\mathbf{L}$ to its *conventional* basis $(\mathbf{a}_i)^T$ as defined in Chapters 2.1 and 9.1 of *IT* A. In this case, the lattice $\mathbf{L}$ may be primitive or centred. If $(\mathbf{a}_i)^T$ forms a primitive basis of $\mathbf{L}$, *i.e.* if $\mathbf{L}$ is primitive, then the basis $(\mathbf{a}_j^*)$ forms a primitive basis of $\mathbf{L}^*$. If $\mathbf{L}$ is centred, *i.e.* $(\mathbf{a}_i)^T$ is not a primitive basis of $\mathbf{L}$, then there exists a centring matrix $\boldsymbol{P}$, $0 < \det(\boldsymbol{P}) < 1$, by which three linearly independent vectors of $\mathbf{L}$ with rational coefficients are generated from those with integer coefficients, *cf. IT* A, Table 5.1.

Moreover, $\boldsymbol{P}$ can be chosen such that the set of vectors

$$(\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3)^T = (\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3)^T\boldsymbol{P} \qquad (1.5.3.8)$$

forms a primitive basis of $\mathbf{L}$. Then the basis vectors $(\mathbf{p}_1^*, \mathbf{p}_2^*, \mathbf{p}_3^*)$ of the lattice reciprocal to the lattice generated by $(\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3)^T$ are determined by

$$(\mathbf{p}_1^*, \mathbf{p}_2^*, \mathbf{p}_3^*) = \boldsymbol{P}^{-1}(\mathbf{a}_1^*, \mathbf{a}_2^*, \mathbf{a}_3^*) \qquad (1.5.3.9)$$

and form a primitive basis of $\mathbf{L}^*$.

Because $\det(\boldsymbol{P}^{-1}) > 1$, not all vectors $\mathbf{K}$ of the form (1.5.3.7) belong to $\mathbf{L}^*$. If k_1, k_2, k_3 are the (integer) coefficients of these vectors $\mathbf{K}$ referred to $(\mathbf{a}_j^*)$ and $k_{p1}\mathbf{p}_1^* + k_{p2}\mathbf{p}_2^* + k_{p3}\mathbf{p}_3^*$ are the vectors of $\mathbf{L}^*$, then $\mathbf{K} = (k_j)^T(\mathbf{a}_j^*) = (k_j)^T\boldsymbol{P}(\mathbf{p}_i^*) = (k_{pi})^T(\mathbf{p}_i^*)$ is a vector of $\mathbf{L}^*$ if and only if the coefficients

$$(k_{p1}, k_{p2}, k_{p3})^T = (k_1, k_2, k_3)^T\boldsymbol{P} \qquad (1.5.3.10)$$

are integers. In other words, $(k_1, k_2, k_3)^T$ has to fulfil the equation

$$(k_1, k_2, k_3)^T = (k_{p1}, k_{p2}, k_{p3})^T\boldsymbol{P}^{-1}. \qquad (1.5.3.11)$$

As is well known, the Bravais type of the reciprocal lattice $\mathbf{L}^*$ is not necessarily the same as that of its direct lattice $\mathbf{L}$. If $\boldsymbol{W}$ is the matrix of a (point-) symmetry operation of the direct lattice, referred to its basis $(\mathbf{a}_i)^T$, then $\boldsymbol{W}^{-1}$ is the matrix of the same symmetry operation of the reciprocal lattice but referred to the dual basis $(\mathbf{a}_i^*)$. This does not affect the symmetry because in a (symmetry) group the inverse of each element in the group also belongs to the group. Therefore, the (point) symmetries of a lattice

† In crystallography vectors are designated by small bold-faced letters. With $\mathbf{K}$ we make an exception in order to follow the tradition of physics. A crystallographic alternative would be $\mathbf{t}^*$.

‡ The lattice $\mathbf{L}$ is often called the *direct lattice*. These names are historically introduced and cannot be changed, although equations (1.5.3.5) and (1.5.3.6) show that essentially neither of the lattices is preferred: they form a pair of *mutually reciprocal* lattices.

and its reciprocal lattice are always the same. However, there may be differences in the matrix descriptions due to the different orientations of $\mathbf{L}$ and $\mathbf{L}^*$ relative to the symmetry elements of $\bar{\mathcal{G}}$ and due to the reference to the different bases $(\mathbf{a}_i)^T$ and $(\mathbf{a}_i^*)$. For example, if $\mathbf{L}$ has the point symmetry (Hermann–Mauguin symbol) $\bar{3}m1$, then the symbol for the point symmetry of $\mathbf{L}^*$ is $\bar{3}1m$ and *vice versa*.

1.5.3.4. *Irreducible representations of space groups and the reciprocal-space group*

Let $(\mathbf{a}_i)^T$ be a conventional basis of the lattice $\mathbf{L}$ of the space group $\mathcal{G}$. From (1.5.3.6), $k_i = q_i/N_i$ and $\mathbf{k} = \sum_{k=1}^{3} k_i \mathbf{a}_i^*$, equation (1.5.3.4) can be written

$$\Gamma^{q_1 q_2 q_3}[(\boldsymbol{I},\boldsymbol{t})] = \Gamma^{\mathbf{k}}[(\boldsymbol{I},\boldsymbol{t})] = \exp[-i\mathbf{k}\cdot\mathbf{t}]. \qquad (1.5.3.12)$$

Equation (1.5.3.12) has the same form if a primitive basis $(\mathbf{p}_i)^T$ of $\mathbf{L}$ has been chosen. In this case, the vector $\mathbf{k}$ is given by $\mathbf{k} = \sum_{i=1}^{3} k_{pi}\mathbf{p}_i^*$.

Let a primitive basis $(\mathbf{p}_i)^T$ be chosen for the lattice $\mathbf{L}$. The set of all vectors $\mathbf{k}$ (known as wavevectors) forms a discontinuous array. Consider two wavevectors $\mathbf{k}$ and $\mathbf{k}' = \mathbf{k} + \mathbf{K}$, where $\mathbf{K}$ is a vector of the reciprocal lattice $\mathbf{L}^*$. Obviously, $\mathbf{k}$ and $\mathbf{k}'$ describe the same irrep of $\mathcal{T}$. Therefore, to determine all irreps of $\mathcal{T}$ it is necessary to consider only the wavevectors of a small region of the reciprocal space, where the translation of this region by all vectors of $\mathbf{L}^*$ fills the reciprocal space without gap or overlap. Such a region is called a *fundamental region* of $\mathbf{L}^*$. (The nomenclature in literature is not quite uniform. We follow here widely adopted definitions.)

The fundamental region of $\mathbf{L}^*$ is not uniquely determined. Two types of fundamental regions are of interest in this chapter:

(1) The *first Brillouin zone* is that range of $\mathbf{k}$ space around $\mathbf{o}$ for which $|\mathbf{k}| \leq |\mathbf{K} - \mathbf{k}|$ holds for any vector $\mathbf{K} \in \mathbf{L}^*$ (*Wigner–Seitz cell* or *domain of influence* in $\mathbf{k}$ space). The Brillouin zone is used in books and articles on irreps of space groups.

(2) The *crystallographic unit cell in reciprocal space*, for short *unit cell*, is the set of all $\mathbf{k}$ vectors with $0 \leq k_i < 1$. It corresponds to the unit cell used in crystallography for the description of crystal structures in direct space.

Let $\mathbf{k}$ be some vector according to (1.5.3.12) and $\boldsymbol{W}$ be the matrices of $\bar{\mathcal{G}}$. The following definitions are useful:

Definition. The set of all vectors $\mathbf{k}'$ fulfilling the condition

$$\mathbf{k}' = \mathbf{k}\boldsymbol{W} + \mathbf{K}, \quad \boldsymbol{W} \in \bar{\mathcal{G}}, \quad \mathbf{K} \in \mathbf{L}^* \qquad (1.5.3.13)$$

is called *the orbit of* $\mathbf{k}$.

Definition. The set of all matrices $\boldsymbol{W} \in \bar{\mathcal{G}}$ for which

$$\mathbf{k} = \mathbf{k}\boldsymbol{W} + \mathbf{K}, \quad \mathbf{K} \in \mathbf{L}^* \qquad (1.5.3.14)$$

forms a group which is called the *little co-group* $\bar{\mathcal{G}}^{\mathbf{k}}$ of $\mathbf{k}$. The vector $\mathbf{k}$ is called *general* if $\bar{\mathcal{G}}^{\mathbf{k}} = \{\boldsymbol{I}\}$; otherwise $\bar{\mathcal{G}}^{\mathbf{k}} > \{\boldsymbol{I}\}$ and $\mathbf{k}$ is called *special*.

The little co-group $\bar{\mathcal{G}}^{\mathbf{k}}$ is a subgroup of the point group $\bar{\mathcal{G}}$. Consider the coset decomposition of $\bar{\mathcal{G}}$ relative to $\bar{\mathcal{G}}^{\mathbf{k}}$.

Definition. If $\{\boldsymbol{W}_m\}$ is a set of coset representatives of $\bar{\mathcal{G}}$ relative to $\bar{\mathcal{G}}^{\mathbf{k}}$, then the set $\{\mathbf{k}\boldsymbol{W}_m\}$ is called the *star* of $\mathbf{k}$ and the vectors $\mathbf{k}\boldsymbol{W}_m$ are called the *arms of the star*.

The number of arms of the star of $\mathbf{k}$ is equal to the order $|\bar{\mathcal{G}}|$ of the point group $\bar{\mathcal{G}}$ divided by the order $|\bar{\mathcal{G}}^{\mathbf{k}}|$ of the symmetry group $\bar{\mathcal{G}}^{\mathbf{k}}$ of $\mathbf{k}$. If $\mathbf{k}$ is general, then there are $|\bar{\mathcal{G}}|$ vectors from the orbit of $\mathbf{k}$ in each fundamental region and $|\bar{\mathcal{G}}|$ arms of the star. If $\mathbf{k}$ is special with little co-group $\bar{\mathcal{G}}^{\mathbf{k}}$, then the number of arms of the star of $\mathbf{k}$ and the number of $\mathbf{k}$ vectors in the fundamental region from the orbit of $\mathbf{k}$ is $|\bar{\mathcal{G}}\,|/|\bar{\mathcal{G}}^{\mathbf{k}}|$.

Definition. The group of all elements $(\boldsymbol{W},\boldsymbol{w}) \in \mathcal{G}$ for which $\boldsymbol{W} \in \bar{\mathcal{G}}^{\mathbf{k}}$ is called the *little group* $\mathcal{L}^{\mathbf{k}}$ *of* $\mathbf{k}$.

Equation (1.5.3.14) for $\mathbf{k}$ resembles the equation

$$\boldsymbol{x} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{t}, \quad \mathbf{t} \in \mathbf{L} \qquad (1.5.3.15)$$

by which the fixed points of the symmetry operation $(\boldsymbol{W},\boldsymbol{t})$ of a symmorphic space group $\mathcal{G}_0$ are determined. Indeed, the orbits of $\mathbf{k}$ defined by (1.5.3.13) correspond to the point orbits of $\mathcal{G}_0$, the little co-group $\bar{\mathcal{G}}^{\mathbf{k}}$ of $\mathbf{k}$ corresponds to the site-symmetry group of that point $\boldsymbol{X}$ whose coordinates (x_i) have the same values as the vector coefficients $(k_i)^T$ of $\mathbf{k}$, and the star of $\mathbf{k}$ corresponds to a set of representatives of $\boldsymbol{X}$ in $\mathcal{G}_0$. (The analogue of the little group $\mathcal{L}^{\mathbf{k}}$ is rarely considered in crystallography.)

All symmetry operations of $\mathcal{G}_0$ may be obtained as combinations of an operation that leaves the origin fixed with a translation of $\mathbf{L}$, *i.e.* are of the kind $(\boldsymbol{W},\boldsymbol{t}) = (\boldsymbol{I},\boldsymbol{t})(\boldsymbol{W},\boldsymbol{o})$. We now define the analogous group for the $\mathbf{k}$ vectors. Whereas $\mathcal{G}_0$ is a realization of the corresponding abstract group in direct (point) space, the group to be defined will be a realization of it in reciprocal (vector) space.

Definition. The group $\mathcal{G}^*$ which is the semidirect product of the point group $\bar{\mathcal{G}}$ and the translation group of the reciprocal lattice $\mathbf{L}^*$ of $\mathcal{G}$ is called the *reciprocal-space group of* $\mathcal{G}$.

The elements of $\mathcal{G}^*$ are the operations $(\boldsymbol{W},\boldsymbol{K}) = (\boldsymbol{I},\boldsymbol{K})(\boldsymbol{W},\boldsymbol{o})$ with $\boldsymbol{W} \in \bar{\mathcal{G}}$ and $\mathbf{K} \in \mathbf{L}^*$. In order to emphasize that $\mathcal{G}^*$ is a group acting on reciprocal space and not the inverse of a space group (whatever that may mean) we insert a hyphen '-' between 'reciprocal' and 'space'.

From the definition of $\mathcal{G}^*$ it follows that space groups of the same type define the same type of reciprocal-space group $\mathcal{G}^*$. Moreover, as $\mathcal{G}^*$ does not depend on the column parts of the space-group operations, all space groups of the same arithmetic crystal class determine the same type of $\mathcal{G}^*$; for arithmetic crystal class see Section 1.5.3.2. Following Wintgen (1941), the types of reciprocal-space groups $\mathcal{G}^*$ are listed for the arithmetic crystal classes of space groups, *i.e.* for all space groups $\mathcal{G}$, in Appendix 1.5.1.

1.5.4. Conventions in the classification of space-group irreps

Because of the isomorphism between the reciprocal-space groups $\mathcal{G}^*$ and the symmorphic space groups $\mathcal{G}_0$ one can introduce crystallographic conventions in the classification of space-group irreps. These conventions will be compared with those which have mainly been used up to now. Illustrative examples to the following more theoretical considerations are discussed in Section 1.5.5.1.

1.5.4.1. *Fundamental regions*

Different types of regions of reciprocal space may be chosen as fundamental regions, see Section 1.5.3.4. The most frequently used type is the first Brillouin zone, which is the Wigner–Seitz cell (or Voronoi region, Dirichlet domain, domain of influence; *cf. IT* A, Chapter 9.1) of the reciprocal lattice. It has the property that with each $\mathbf{k}$ vector also its star belongs to the Brillouin zone. Such a choice has three advantages:

(1) the Brillouin zone is always primitive and it manifests the point symmetry of the reciprocal lattice $\mathbf{L}^*$ of $\mathcal{G}$;