posed. 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 5.1.3.1.

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

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

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

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

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

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

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

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

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 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 $\overline{\mathcal{G}}$ 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) $\overline{3}m1$, then the symbol for the point symmetry of $\mathbf{L}^*$ is $\overline{3}1m$ 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

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

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 $\mathbf{k} = \sum_{i=1}^{3} k_{pi}\mathbf{p}_i^*$ with rational coefficients k_{pi}.

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). Visually, it is the region of endpoints of the $\mathbf{k}$ vectors that are nearer to the origin than to any other point of the reciprocal lattice. The Brillouin zone is a centrosymmetric body bounded by centrosymmetric planes which bisect perpendicularly the connecting lines from the origin to the neighbouring reciprocal-lattice points. 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 $\overline{\mathcal{G}}$. The following definitions are useful:

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

$$\mathbf{k}' = \mathbf{k}\boldsymbol{W} + \mathbf{K}, \quad \boldsymbol{W} \in \overline{\mathcal{G}}, \quad \mathbf{K} \in \mathbf{L}^* \tag{1.5.3.13}$$

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

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

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

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

In words: The $\mathbf{k}$ vector is called *general* if its little co-group $\overline{\mathcal{G}}^{\mathbf{k}}$ is the identity of $\overline{\mathcal{G}}$. Otherwise, $\overline{\mathcal{G}}^{\mathbf{k}}$ is a non-trivial subgroup of the point group $\overline{\mathcal{G}}$ of $\mathcal{G}$, $\overline{\mathcal{G}} > \overline{\mathcal{G}}^{\mathbf{k}}$, and $\mathbf{k}$ is called a *special vector* of the reciprocal space.

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

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

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 $\overline{\mathcal{G}}^{\mathbf{k}}$ 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 $\mathbf{k}$.

Consider the coset decomposition of $\overline{\mathcal{G}}$ relative to $\overline{\mathcal{G}}^{\mathbf{k}}$.

Definition. If $\{\boldsymbol{W}_m\}$ is a set of coset representatives of $\overline{\mathcal{G}}$ relative to $\overline{\mathcal{G}}^{\mathbf{k}}$, 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 $|\overline{\mathcal{G}}|$ of the point group $\overline{\mathcal{G}}$ divided by the order $|\overline{\mathcal{G}}^{\mathbf{k}}|$ of the symmetry group $\overline{\mathcal{G}}^{\mathbf{k}}$ of $\mathbf{k}$. If $\mathbf{k}$ is general, then there are $|\overline{\mathcal{G}}|$ vectors from the orbit of $\mathbf{k}$ in each fundamental region and $|\overline{\mathcal{G}}|$ arms of the star. If $\mathbf{k}$ is special with little co-group $\overline{\mathcal{G}}^{\mathbf{k}}$, 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 $|\overline{\mathcal{G}}|/|\overline{\mathcal{G}}^{\mathbf{k}}|$.

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

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 transla-

tion 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 $\overline{\mathcal{G}}$ and the translation group of the reciprocal lattice $\mathbf{L}^*$ of $\mathcal{G}$ is called the *reciprocal-space group of* $\mathcal{G}$.

By this definition, the reciprocal-space group $(\mathcal{G})^*$ is isomorphic to a symmorphic space group $\mathcal{G}_0$. The elements of $\mathcal{G}_0$ are the operations $(\boldsymbol{W}, \boldsymbol{t}_{\boldsymbol{K}}) = (\boldsymbol{I}, \boldsymbol{t}_{\boldsymbol{K}})(\boldsymbol{W}, \boldsymbol{o})$ with $\boldsymbol{W} \in \overline{\mathcal{G}}$ and $\boldsymbol{t}_{\boldsymbol{K}} \in \mathbf{L}$ with the coefficients of $\mathbf{K}$. 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 A1.5.1.

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.

1.5.4.1. 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. The Brillouin zone has the property of including the star of each $\mathbf{k}$ vector that belongs to it. Such a choice has three advantages:

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

(2) only $\mathbf{k}$ vectors of the boundary of the Brillouin zone may have little-group representations which are obtained from projective representations of the little co-group $\overline{\mathcal{G}}^{\mathbf{k}}$, see *e.g.* BC, p. 156;

(3) for physical reasons, the Brillouin zone may be the most convenient fundamental region.

Of these advantages only the third may be essential. For the classification of irreps the minimal domains, see Section 1.5.4.2, are much more important than the fundamental regions. The minimal domain does not display the point-group symmetry anyway and the distinguished $\mathbf{k}$ vectors always belong to its boundary however the minimal domain may be chosen.

The serious disadvantage of the Brillouin zone is its often complicated shape which, moreover, depends on the lattice parameters of $\mathbf{L}^*$, *cf.* Section 1.5.5.3. The body that represents the Brillouin zone belongs to one of the five Fedorov polyhedra (more or less distorted versions of the cubic forms cube, rhombdodecahedron or cuboctahedron, of the hexagonal prism, or of the tetragonal elongated rhombdodecahedron). A more detailed description is that by the 24 *symmetrische Sorten* (Delaunay sorts) of Delaunay (1933*a*,*b*), Figs. 11 and 12. According to this classification, the Brillouin zone may display three types of polyhedra of cubic, one type of hexagonal, two of rhombohedral, three of tetragonal, six of orthorhombic, six of monoclinic, and three types of triclinic symmetry.

For low symmetries the shape of the Brillouin zone is so variable that BC, p. 90 *ff.* chose a primitive unit cell of $\mathbf{L}^*$ for the fundamental regions of triclinic and monoclinic crystals. This cell also reflects the point symmetry of $\mathbf{L}^*$, it has six faces only, and although its shape varies with the lattice parameters all cells are affinely equivalent. For space groups of higher symmetry, BC and most other authors prefer the Brillouin zone.

Considering $\mathbf{L}^*$ as a lattice, one can refer it to its conventional crystallographic lattice basis. Referred to this basis, the *unit cell of* $\mathbf{L}^*$ is always an alternative to the Brillouin zone. With the exception of the hexagonal lattice, the unit cell of $\mathbf{L}^*$ reflects the point symmetry, it has only six faces and its shape is always affinely equivalent for varying lattice parameters. For a space group $\mathcal{G}$ with a primitive lattice, the above-defined conventional unit cell of $\mathbf{L}^*$ is also primitive. If $\mathcal{G}$ has a centred lattice, then $\mathbf{L}^*$ also belongs to a type of centred lattice and the *conventional* cell of $\mathbf{L}^*$ [not to be confused with the cell spanned by the basis $(\mathbf{a}_j^*)$ dual to the basis $(\mathbf{a}_i)^T$] is larger than necessary. However, this is not disturbing because in this context the fundamental region is an auxiliary construction only for the definition of the minimal domain; see Section 1.5.4.2.

1.5.4.2. Minimal domains

One can show that all irreps of $\mathcal{G}$ can be built up from the irreps $\Gamma^{\mathbf{k}}$ of $\mathcal{T}$. Moreover, to find all irreps of $\mathcal{G}$ it is only necessary to consider one $\mathbf{k}$ vector from each orbit of $\mathbf{k}$, *cf.* CDML, p. 31.

Definition. A simply connected part of the fundamental region which contains *exactly one* $\mathbf{k}$ vector of each orbit of $\mathbf{k}$ is called a *minimal domain* Φ.

The choice of the minimal domain is by no means unique. One of the difficulties in comparing the published data on irreps of space groups is due to the different minimal domains found in the literature.

The number of $\mathbf{k}$ vectors of each general $\mathbf{k}$ orbit in a fundamental region is always equal to the order of the point group $\overline{\mathcal{G}}$ of $\mathcal{G}$; see Section 1.5.3.4. Therefore, the volume of the minimal domain Φ in reciprocal space is $1/|\overline{\mathcal{G}}|$ of the volume of the fundamental region. Now we can restrict the search for all irreps of $\mathcal{G}$ to the $\mathbf{k}$ vectors within a minimal domain Φ.

In general, in representation theory of space groups the Brillouin zone is taken as the fundamental region and Φ is called a *representation domain*.[4] Again, the volume of a representation domain in reciprocal space is $1/|\overline{\mathcal{G}}|$ of the volume of the Brillouin zone. In addition, as the Brillouin zone contains for each $\mathbf{k}$ vector all $\mathbf{k}$ vectors of the star of $\mathbf{k}$, by application of all symmetry operations $\boldsymbol{W} \in \overline{\mathcal{G}}$ to Φ one obtains the Brillouin zone; *cf.* BC, p. 147. As the Brillouin zone may change its geometrical type depending on the lattice parameters, the type of the representation domain may also vary with varying lattice parameters; see the examples of Section 1.5.5.

The simplest crystal structures are the lattice-like structures that are built up of translationally equivalent points (centres of particles) only. For such a structure the point group $\overline{\mathcal{G}}$ of the space group $\mathcal{G}$ is equal to the point group $\mathcal{Q}$ of its lattice $\mathbf{L}$. Such point groups are called *holohedral*, the space group $\mathcal{G}$ is called *holo-*

[4] From definition 3.7.1 on p. 147 of BC, it does not follow that a representation domain contains *exactly one* $\mathbf{k}$ vector from each star. The condition 'The intersection of the representation domain with its symmetrically equivalent domains is empty' is missing. Lines 14 to 11 from the bottom of p. 149, however, state that such a property of the representation domain is intended. The representation domains of CDML, Figs. 3.15–3.29 contain *at least one* $\mathbf{k}$ vector of each star (Vol. 1, pp. 31, 57 and 65). On pp. 66, 67 a procedure is described for eliminating those $\mathbf{k}$ vectors from the representation domain which occur more than once. In the definition of Altmann (1977), p. 204, the representation domain contains *exactly one* arm (prong) per star.