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 $|\mathbf{k}| \le |\mathbf{K} - \mathbf{k}|$ 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 $0 \le k_i < 1$. 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 $\mathcal{G}$;

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