To each space group $\mathcal{G}$ belongs an infinite set $\mathcal{T}$ of translations, the *translation subgroup* of $\mathcal{G}$. The group $\mathcal{T}$ 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 symmetry operations, *i.e.* the elements g: $\tilde{\boldsymbol{x}} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{w}$ 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 right cosets relative to $\mathcal{T}$:

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

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 $\boldsymbol{I}$ is the unit matrix and $\boldsymbol{o}$ 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 $\overline{\mathcal{G}}$ in books on representation theory) describing the symmetry of the external shape of the macroscopic crystal and being represented by the matrices $\boldsymbol{W}_1, \boldsymbol{W}_2, \ldots, \boldsymbol{W}_n$, $\mathcal{P} = \{\boldsymbol{W}_i\}$. 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 $\mathcal{G}_0$. (For the term 'site-symmetry group', see Section 1.5.4.2.)

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 8.2.3; see also Section 8.3.4 and Table 8.3.4.1.

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, assuming the Born–von Karman boundary conditions

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

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 $(\boldsymbol{I}, \boldsymbol{t})$,

$$(\boldsymbol{I}, \boldsymbol{N}\boldsymbol{t}) = (\boldsymbol{I}, \boldsymbol{o}) \quad (1.5.3.3)$$

holds, where $\boldsymbol{N}\boldsymbol{t}$ 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 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

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

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):

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

In the present chapter only the physicist's basis of the reciprocal lattice is employed, and hence the use of $\mathbf{a}_i^*$ should not lead to misunderstandings. The set of all vectors $\mathbf{K}$,[2]

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

k_i integer, is called the lattice reciprocal to $\mathbf{L}$ or the *reciprocal lattice* $\mathbf{L}^*$.[3]

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 trans-

[2] See Note (1) in Section 1.5.1.

[3] 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.

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

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

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 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

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

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

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

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

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

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

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

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

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