1.5. CLASSIFICATION OF SPACE-GROUP REPRESENTATIONS

tion of **L**, *i.e.* are of the kind $(W, t) = (I, t)(W, o)$. We now define the analogous group for the **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 **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 $(W, t_K) = (I, t_K)(W, o)$ with $W \in \overline{\mathcal{G}}$ and $t_K \in \mathbf{L}$ with the coefficients of **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 **k** vector that belongs to it. Such a choice has three advantages:

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

(2) only **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 **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 **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 **L*** for the fundamental regions of triclinic and monoclinic crystals. This cell also reflects the point symmetry of **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 **L*** as a lattice, one can refer it to its conventional crystallographic lattice basis. Referred to this basis, the *unit cell of* **L*** is always an alternative to the Brillouin zone. With the exception of the hexagonal lattice, the unit cell of **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 **L*** is also primitive. If $\mathcal{G}$ has a centred lattice, then **L*** also belongs to a type of centred lattice and the *conventional* cell of **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 **k** vector from each orbit of **k**, *cf.* CDML, p. 31.

Definition. A simply connected part of the fundamental region which contains *exactly one* **k** vector of each orbit of **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 **k** vectors of each general **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 **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 **k** vector all **k** vectors of the star of **k**, by application of all symmetry operations $W \in \overline{\mathcal{G}}$ 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 **L**. Such point groups are called *holohedral*, the space group $\mathcal{G}$ is called *holo-*

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[4] From definition 3.7.1 on p. 147 of BC, it does not follow that a representation domain contains *exactly one* **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* **k** vector of each star (Vol. 1, pp. 31, 57 and 65). On pp. 66, 67 a procedure is described for eliminating those **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.

references