Mauguin symbols for frieze, rod and layer groups reflects the relationship between reducible space groups and subperiodic groups as their factor groups, see Section 1.2.17. In the case of the layer groups, our choice thus substantially differs from that made by Wood (1964). The interpretation of subperiodic groups as factor groups of reducible space groups also has consequences in the representation theory of space and subperiodic groups. Last but not least, this relationship reveals relations between the algebraic structure of the space group of a crystal and the symmetries of planar sections or of straight lines penetrating the crystal. These relations, analogous to the relations between the point group and symmetries of Wyckoff positions, will be described elsewhere.

It should be noted finally that all the information about scanning can be and is presented in a structure-independent way in terms of the groups involved. The scanning tables therefore extend the standard description of space groups.

5.2.2. The basic concepts of the scanning

If a crystal with a symmetry of the space group $\mathcal{G}$ is transected by a crystallographic[1] plane, called a *section plane*, then the subgroup of all elements of the space group $\mathcal{G}$ which leave the plane invariant is a layer group, which is called a *sectional layer group*, of this section plane under the action of the group $\mathcal{G}$. Analogously, if the crystal is penetrated by a crystallographic[1] straight line, called the *penetration straight line*, then the subgroup of all elements of the space group $\mathcal{G}$ which leave the straight line invariant is a rod group, which is called the *penetration rod group*, of this penetration straight line under the action of the group $\mathcal{G}$.

Sectional layer groups are therefore symmetries of crystallographic section planes and penetration rod groups are symmetries of crystallographic penetration straight lines under the action of space groups. In this sense they are analogous to site symmetries of Wyckoff positions. In addition, analogous to points, the section planes and penetration straight lines form orbits under the action of the space group $\mathcal{G}$. Planes or straight lines belonging to the same orbit have, with reference to their respective coordinate systems, the same sectional layer symmetry or penetration rod symmetry and the crystal is described in the same way with reference to any of these coordinate systems.

While every sectional layer group is, by definition, a subgroup of the corresponding space group, not every subgroup of the space group which is a layer group is necessarily a sectional layer group. Analogously, a penetration rod group is a subgroup of the corresponding space group but not every rod subgroup of a space group is a penetration rod group. It can be shown that every sectional layer group is either a maximal layer subgroup of the space group or a halving subgroup of a maximal layer subgroup, see Section 5.2.2.6.

We shall consider explicitly only the sectional layer groups, although the penetration rod groups can also be deduced from the scanning tables, see the example in Section 5.2.2.2.

5.2.2.1. The scanning for sectional layer groups

A plane in a three-dimensional space is associated with a two-dimensional vector space $V(\mathbf{a}', \mathbf{b}')$ which is called the *orientation* of the plane. If the plane of this orientation also contains a point $P + \mathbf{r}$, we shall denote it by a symbol $(P + \mathbf{r}, V(\mathbf{a}', \mathbf{b}'))$. A straight line is associated with a one-dimensional vector space $V(\mathbf{d})$ which is called the *direction* of the straight line. If the straight line of this direction also contains a point $P + \mathbf{r}$, we shall denote it by a symbol $(P + \mathbf{r}, V(\mathbf{d}))$. We assume in what follows that the vector $\mathbf{d}$ is not a linear combination of vectors $\mathbf{a}'$, $\mathbf{b}'$.

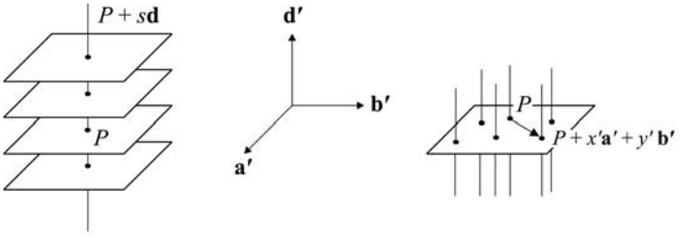

Fig. 5.2.2.1. Sets of parallel planes (left) and sets of parallel straight lines (right).

Then the set of all parallel planes with a common orientation $V(\mathbf{a}', \mathbf{b}')$ contains planes $(P + s\mathbf{d}; V(\mathbf{a}', \mathbf{b}'))$. Points $P + s\mathbf{d}$ along a straight line $(P; V(\mathbf{d}))$ specify the location of individual planes as the points in which the planes intersect with the straight line $(P; V(\mathbf{d}))$ (Fig. 5.2.2.1 left). On the other hand, the set of all straight lines with a common direction $V(\mathbf{d})$ contains straight lines $(P + x'\mathbf{a}' + y'\mathbf{b}'; V(\mathbf{d}))$. The location of individual straight lines of the set is defined by their intersection points $P + x'\mathbf{a}' + y'\mathbf{b}'$ with the plane $(P; V(\mathbf{a}', \mathbf{b}'))$ (Fig. 5.2.2.1 right).

We consider now a space group $\mathcal{G}$, with a point group G and translation subgroup T_G, described by a symmetry diagram or by symmetry operations with reference to a crystallographic coordinate system $(P; \mathbf{a}, \mathbf{b}, \mathbf{c})$ (as listed, for example, in *IT* A). We want to solve the following two problems:

(1) Find the sectional layer groups $\mathcal{L}(P + s\mathbf{d}; V(\mathbf{a}', \mathbf{b}'))$ which contain all those elements of $\mathcal{G}$ which leave the planes $(P + s\mathbf{d}; V(\mathbf{a}', \mathbf{b}'))$ invariant.

(2) Find the orbit of planes, generated by the plane $(P + s\mathbf{d}; V(\mathbf{a}', \mathbf{b}'))$ under the action of the space group $\mathcal{G}$.

The general goal is to describe all possible cases, classify and systemize them. Since the first part of the problem may be described as a search for the change of the sectional layer symmetry as a plane of a given orientation changes its position so that one of its points moves along a straight line $(P; V(\mathbf{d}))$, we shall call this procedure *the scanning of the space group $\mathcal{G}$ for sectional layer groups of planes with the orientation $V(\mathbf{a}', \mathbf{b}')$ along the scanning line* $(P; V(\mathbf{d}))$. We shall use also abbreviated expressions in different contexts; for example *the scanning of the space group $\mathcal{G}$ (for layer groups)* will mean the determination of the sectional layer groups for the space group $\mathcal{G}$ and all possible orientations.

An analogous procedure is *the scanning of the space group $\mathcal{G}$ for penetration rod groups $\mathcal{R}(P + x'\mathbf{a}' + y'\mathbf{b}'; V(\mathbf{d}))$ of straight lines with the direction $V(\mathbf{d})$ along the scanning plane* $(P; V(\mathbf{a}', \mathbf{b}'))$.

Crystallographic orientations of planes are characterized by Miller (or Bravais–Miller) indices (*hkl*) [or (*hkil*)]. These indices determine a two-dimensional vector space, the orientation, all vectors of which leave the section planes with given Miller indices invariant. Those vectors of the translation group T_G (the lattice of $\mathcal{G}$) which lie in this space constitute a two-dimensional translation subgroup $T_{G1} = T(\mathbf{a}', \mathbf{b}')$ with a certain basis $(\mathbf{a}', \mathbf{b}')$. This is the group of all those translations from T_G that leave the section planes with given Miller indices invariant. This group is therefore a common translation subgroup of all sectional layer groups of section planes with these Miller indices. The vectors $\mathbf{a}'$, $\mathbf{b}'$ can be

[1] If the section plane is not crystallographic, its symmetry is not a layer group but either a rod group or a site-symmetry group. If the penetration straight line is not crystallographic, its symmetry is a site-symmetry group.

taken as the basis vectors of the two-dimensional vector space $V(\mathbf{a}', \mathbf{b}')$ and hence $T(\mathbf{a}', \mathbf{b}') = T_G \cap V(\mathbf{a}', \mathbf{b}')$.

The *scanning line* $(P; V(\mathbf{d}))$ and the *scanning direction* $V(\mathbf{d})$ are defined by a vector $\mathbf{d}$. This vector can be, quite generally, chosen as any vector complementary to the orientation $V(\mathbf{a}', \mathbf{b}')$, *i.e.* as an arbitrary vector, noncollinear with $\mathbf{a}'$, $\mathbf{b}'$, which needs not even define a crystallographic direction. Since, for a given space group $\mathcal{G}$ and orientation $V(\mathbf{a}', \mathbf{b}')$, the sectional layer group $\mathcal{L}(P + s\mathbf{d}; V(\mathbf{a}', \mathbf{b}'))$ depends only on the distance of the plane from the origin P, it might seem to be of advantage to choose the direction $\mathbf{d}$ always perpendicular to $V(\mathbf{a}', \mathbf{b}')$, as in the example below. This, however, is not always the most suitable choice. We shall subordinate the choice of vector $\mathbf{d}$ to a strict convention, see Section 5.2.2.3, and call it the *scanning vector*.

Example

Consider a crystal whose space-group symmetry is *Pbcm*, D_{2h}^{11} (No. 57). The sectional layer symmetries of planes with an (001) orientation depend on the location of the plane along the line $P + z\mathbf{c}$, where the basis vector $\mathbf{c}$ is chosen as the *scanning vector* $\mathbf{d}$. If $z = 0, \frac{1}{2}$, the sectional layer group is $p2/b11$ (L16), if $z = \frac{1}{4}, \frac{3}{4}$, the sectional layer group is $pb2_1m$ (L29). The same holds if we add an integer n to the coordinate z. All these layer groups are maximal subgroups of the group *Pbcm*. The sectional layer symmetry of any other plane is a layer group $pb11$ (L12). The symbol of a layer group for a section plane located at $P + z\mathbf{c}$ is given with reference to the coordinate system $(P + z\mathbf{d}; \mathbf{a}, \mathbf{b}, \mathbf{d} = \mathbf{c})$. Notice that there are an infinite number of section planes with $z = n$ and $(n + \frac{1}{2})$ or $z = (n + \frac{1}{4})$ and $(n + \frac{3}{4})$ and an infinite number of corresponding sectional layer groups which can be written as $p2/b11$ $(n\mathbf{d})$ and $p2/b11$ $[(n + \frac{1}{2})\mathbf{d}]$ (L16) or $pb2_1m$ $[(n + \frac{1}{4})\mathbf{d}]$ and $pb2_1m$ $[(n + \frac{3}{4})\mathbf{d}]$ (L29) with reference to the coordinate system $(P; \mathbf{a}, \mathbf{b}, \mathbf{d} = \mathbf{c})$. All these groups are maximal layer subgroups of the group *Pbcm*. There are also an infinite number of section planes with other values of z which change continuously between the previously given discrete values of z; to all these section planes there corresponds one sectional layer group, $pb11$ (L12), whose Hermann–Mauguin symbol does not depend on z. This group is said to be *floating* in the direction $\mathbf{c}$ and it is a halving subgroup of all previously given sectional layer groups, see Section 5.2.2.6.

5.2.2.2. The scanning group and the scanning theorem

The main step in the solution of the scanning problem and in its tabular presentation is the introduction of the *scanning group* (Kopský, 1990), which is a central concept of scanning. This group is an intermediate product in the process for scanning of the sectional layer groups and for the penetration rod groups. We shall introduce this group with reference to the scanning for sectional layer groups. The scanning group is then a space group which depends on the *scanned* space group $\mathcal{G}$ and on the orientation $V(\mathbf{a}', \mathbf{b}')$. The prominent status of the scanning group is seen from: (i) the *scanning theorem*, which facilitates determination of the sectional layer groups as well as penetration rod groups in more complicated cases, and (ii) the convention for the choice of vectors $\mathbf{a}'$, $\mathbf{b}'$ and $\mathbf{d}$, see Section 5.2.2.3, which standardizes the description of the scanning.

Definition of the scanning group: Let $\mathcal{G}$ be a space group with a point group G and $V(\mathbf{a}', \mathbf{b}')$ an orientation of planes, defined by Miller indices (hkl). Further let H be that subgroup of the point group G of the space group $\mathcal{G}$ that contains all those elements of G that leave the orientation $V(\mathbf{a}', \mathbf{b}')$ invariant, so that $HV(\mathbf{a}', \mathbf{b}') = V(\mathbf{a}', \mathbf{b}')$.

The space group

$$\mathcal{H} = \mathcal{H}(\mathcal{G}, (hkl)) = \mathcal{H}(\mathcal{G}, V(\mathbf{a}', \mathbf{b}')), \tag{5.2.2.1}$$

which is an *equitranslational* subgroup of the space group $\mathcal{G}$ corresponding to the point group H, is called the *scanning group* for the space group $\mathcal{G}$ and for the orientation $V(\mathbf{a}', \mathbf{b}')$ with Miller indices (hkl).

The importance of the scanning group for the scanning process is due to the following theorem (Kopský, 1990):

The scanning theorem: The scanning of the space group $\mathcal{G}$ for the sectional layer groups of section planes with an orientation $V(\mathbf{a}', \mathbf{b}')$ is identical with the scanning of the scanning group $\mathcal{H}(\mathcal{G}, (hkl)) = \mathcal{H}(\mathcal{G}, V(\mathbf{a}', \mathbf{b}'))$ for the sectional layer groups of section planes with the same orientation $V(\mathbf{a}', \mathbf{b}')$.

The scanning group $\mathcal{H}$ has, by definition, the same lattice T_G as the scanned group $\mathcal{G}$. However, the scanning group frequently belongs to a lower system than the group $\mathcal{G}$, because its point group H is a subgroup of the point group G, and its conventional basis may be different from the conventional basis of $\mathcal{G}$. In addition, the scanning group is always a *reducible* space group (Kopský, 1988, 1989*a*,*b*, 1990) because its point group H leaves the subspace $V(\mathbf{a}', \mathbf{b}')$ invariant.

Example

Consider the cubic space group $P432$ (O^1) and section planes of orientation defined by the Miller indices (001). The scanning group for this orientation is the group $P422$ (D_4^1) with reference to a basis $\mathbf{a}' = \mathbf{a}$, $\mathbf{b}' = \mathbf{b}$, $\mathbf{d} = \mathbf{c}$. Compare, in Part 6, Table $P432$ (O^1), the blocks headed *Linear orbit* and *Sectional layer group* $\mathcal{L}(s\mathbf{d})$ for the original scanned group and for the scanning group to see that they are identical. Moreover, we receive the same results for orientations defined by the Miller indices (100) and (010) where the scanning group is denoted by the same Hermann–Mauguin symbol $P422$ with reference to appropriate bases.

In addition, the diagram of the scanning group provides immediate information about the penetration rod groups of penetration straight lines with the direction $\mathbf{c}$ characterized by the direction indices [001]. Indeed, the spatial distribution of these rod groups is immediately seen from the diagram of the scanning group $P422$ in the basis $(\mathbf{a}, \mathbf{b}, \mathbf{c})$. For directions corresponding to the indices [100] and [010] we obtain the same results with reference to respective bases $(\mathbf{b}, \mathbf{c}, \mathbf{a})$ and $(\mathbf{c}, \mathbf{a}, \mathbf{b})$.

5.2.2.3. The conventional basis of the scanning group

In the *Scanning tables* of Part 6, we follow the usual crystallographic practice to define the orientation of planes by their Miller indices (Bravais–Miller indices in hexagonal cases). This itself already guarantees that the orientations considered are crystallographic. The choice of vectors $\mathbf{a}'$, $\mathbf{b}'$ and $\mathbf{d}$ is governed by a convention in which we distinguish the cases of orthogonal and inclined scanning.

Convention: Given the orientation of planes by Miller or Bravais–Miller indices, we choose vectors $\mathbf{a}'$, $\mathbf{b}'$ and the vector $\mathbf{d}$ of the scanning direction according to the following rules:

(i) *Orthogonal scanning*: If the scanning group $\mathcal{H}$ is of orthorhombic or higher symmetry, or if it is monoclinic with the

direction of its unique axis orthogonal to the orientation of the planes, we call the scanning *orthogonal* and the vectors $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{d}$ are chosen in such a way that the triplet $(\mathbf{a}', \mathbf{b}', \mathbf{d})$ constitutes a conventional right-handed basis of the scanning group $\mathcal{H}$.

(ii) *Inclined scanning*: If the scanning group is either triclinic or monoclinic with its unique axis parallel to the section planes, we call the scanning *inclined*. In this case we choose vectors $\mathbf{a}'$, $\mathbf{b}'$ in such a way that they constitute a conventional basis of the vector lattice $T(\mathbf{a}', \mathbf{b}')$, common to all sectional layer groups, while the scanning vector $\mathbf{d}$ is chosen as the shortest complementary vector.

Note that, in cases of orthogonal scanning, the first two vectors $\mathbf{a}'$, $\mathbf{b}'$ of the conventional basis of the scanning group $\mathcal{H}$ automatically constitute a conventional basis of the lattice $T(\mathbf{a}', \mathbf{b}')$ and $\mathbf{d}$ is orthogonal to the orientation $V(\mathbf{a}', \mathbf{b}')$. In cases of inclined scanning it is always possible to choose the vectors $\mathbf{a}'$, $\mathbf{b}'$ so that they constitute a conventional basis of the vector lattice $T(\mathbf{a}', \mathbf{b}')$. However, it is generally impossible to choose all three vectors $\mathbf{a}'$, $\mathbf{b}'$ and $\mathbf{d}$ as a strictly conventional basis of the scanning group because the first two vectors must lie in the space defined by Miller (Bravais–Miller) indices, which usually leads to a clash with the metric conditions as they are given, for example, in Section 9.1.4 (vi) and (vii) of *IT* A (2005).

The choice of the scanning direction $\mathbf{d}$ as that of a vector of the basis of the scanning group guarantees the periodicity $\mathbf{d}$ of the scanning. As a result, it is sufficient to describe the scanning for a given orientation, *i.e.* the sectional layer groups and orbits of planes, only in the interval with $0 \leq s < 1$ on the scanning line $P + s\mathbf{d}$. Indeed, the crystal structure of symmetry $\mathcal{G}$ is periodically repeated with periodicity $\mathbf{d}$ in the scanning direction. The sectional layer groups are, however, repeated in the scanning direction with the periodicity of the translation normalizer of $\mathcal{G}$. This is identical with the periodicity of the translation normalizer of the scanning group $\mathcal{H}$ (see the examples in Section 5.2.5.1). We recall that the translation normalizer of the space group $\mathcal{G}$, as defined by Kopský (1993*b*,*c*), is the translation subgroup of the Cheshire group (Euclidean normalizer) of $\mathcal{G}$ [see Hirschfeld (1968) and Koch & Fischer in Part 15 of *IT* A, 1987 edition or later].

In the application of the convention we note the following:

Item 1. If $G = H$ for a certain orientation of planes so that this orientation is invariant under all elements of the point group G of the space group $\mathcal{G}$, then $\mathcal{G} = \mathcal{H}$, *i.e.* the scanning group $\mathcal{H}$ coincides with the original space group $\mathcal{G}$.

The typical cases of this relationship are orientations (001) for the monoclinic, orthorhombic and tetragonal groups and the orientations (0001) for the trigonal and hexagonal groups. In these cases, the conventional basis of the original space group $\mathcal{G}$ also coincides with the conventional basis of the scanning group $\mathcal{H}$ and the group $\mathcal{H}$ is therefore represented by the same Hermann–Mauguin symbol as the group $\mathcal{G}$.

Item 2. The conventional basis of the scanning group $\mathcal{H}$ may differ from the conventional basis of the original group $\mathcal{G}$ even if these groups are identical. In this case the group is generally denoted by different Hermann–Mauguin symbols. This always happens in the cases of monoclinic and very frequently in cases of orthorhombic groups for other orientations than (001) because the conventional vectors $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{d}$ of the scanning group $\mathcal{H}$ cannot be made identical with the conventional basis vectors $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ of the group $\mathcal{G}$.

Example

Consider the space group $\mathcal{G} = Pmmm$ (D_{2h}^1) and the orientations described by the Miller indices (001), (100), (010). The scanning group $\mathcal{H} = \mathcal{G}$ is identical with the scanned group and its Hermann–Mauguin symbol *Pmmm* is the same for all three orientations.

If, however, the scanned group is the group $\mathcal{G} = Pmma$ (D_{2h}^5), then again the scanning group $\mathcal{H}$ is identical with the scanned group $\mathcal{G}$ for the three orientations, but the Hermann–Mauguin symbols of the scanning group are now different: they are *Pmma*, *Pmcm* and *Pbmm* for the orientations (001), (100) and (010), respectively.

Item 3. If $H \subset G$, so that the point group H is a proper subgroup of the point group G, then the conventional basis of the scanning group $\mathcal{H}$ is usually different from the conventional basis of the original group $\mathcal{G}$, although the groups are equitranslational, *i.e.* have the same translation subgroup. The conventional basis of the scanning group $\mathcal{H}$ in the case when $H \subset G$ actually coincides with the conventional basis of the space group $\mathcal{G}$ only in the cases of the orientations (001), (100) and/or (010) if $\mathcal{G}$ is cubic of lattice type P or I and hence $\mathcal{H}$ is tetragonal of the same lattice type. The centring type of the scanning group $\mathcal{H}$ is also frequently different from the centring type of the original group $\mathcal{G}$.

5.2.2.4. The types of scanning

It is useful to characterize various scanning tasks using the names of the crystallographic systems of the scanned group and of the scanning group. The scanning tables are naturally built up from lower to higher symmetries, according to the standard sequence of space groups. In this process, some already-considered space groups of lower crystallographic systems appear as scanning groups for those orientations which are not invariant under the point group G of the scanned space group $\mathcal{G}$ of a higher crystallographic system. In the first column of Table 5.2.2.1, the crystallographic systems are listed in their usual hierarchy and to the right of each system are listed the lower systems from which some groups appear as scanning groups. We use terms such as *tetragonal/monoclinic* scanning when a tetragonal space group $\mathcal{G}$ is considered and the scanning group $\mathcal{H}$ is monoclinic. Simple expressions such as *orthorhombic* scanning will mean that the scanning group $\mathcal{H}$ is orthorhombic, to distinguish it from the expression *scanning of orthorhombic groups*, which means that the original space group $\mathcal{G}$ is orthorhombic. The lattice of trigonal scanning groups in the case of *cubic/trigonal* scanning is always rhombohedral as indicated in parentheses.

Table 5.2.2.1. *Various types of scanning*

Triclinic					
Monoclinic	triclinic				
Orthorhombic	monoclinic	triclinic			
Tetragonal	orthorhombic	monoclinic	triclinic		
Trigonal	orthorhombic	monoclinic	triclinic		
Hexagonal	orthorhombic	monoclinic	triclinic		
Cubic	tetragonal	trigonal (rhombohedral)	orthorhombic	monoclinic	triclinic

5.2.2.5. Orientation orbits

The point group G of the scanned group $\mathcal{G}$ acts on the orientations defined by Miller indices (*hkl*) or Bravais–Miller indices (*hkil*). The set of all orientations $V(\mathbf{a}_i', \mathbf{b}_i')$ obtained from a given orientation $V(\mathbf{a}_1', \mathbf{b}_1')$ by the action of the elements of the group G is called the *orientation orbit*. The point group $H_1 \subseteq G$ which leaves the orientation $V(\mathbf{a}_1', \mathbf{b}_1')$ invariant is the point group of the scanning group $\mathcal{H}_1$ for this orientation. From the coset resolution

$$G = H_1 \cup g_2 H_1 \cup \ldots \cup g_p H_1 \qquad (5.2.2.2)$$

we obtain orientations of the orbit by the action of cosets on the first orientation: $V(\mathbf{a}_i', \mathbf{b}_i') = g_i H_1 V(\mathbf{a}_1', \mathbf{b}_1') = g_i V(\mathbf{a}_1', \mathbf{b}_1')$. In general, the number of orientations in the orbit is equal to the index $p = [G : H_1]$ of the subgroup H_1 in G. The point group $H_i \subset G$ which leaves the orientation $V(\mathbf{a}_i', \mathbf{b}_i')$ invariant is the conjugate subgroup $H_i = g_i H_1 g_i^{-1}$ of the point group H_1 in the group G. If $H_1 = H = G$, then the scanning group $\mathcal{H}$ is identical with the scanned group $\mathcal{G}$ and the orientation orbit contains just one orientation.

In the general case, to each orientation $V(\mathbf{a}_i', \mathbf{b}_i')$ there corresponds a scanning group $\mathcal{H}_i$, conjugate to the scanning group $\mathcal{H}_1$. The elements of a coset $g_i H_1$ send the scanning vector $\mathbf{d}_1$ for the first orientation into scanning vectors $\mathbf{d}_i = g_i H_1 \mathbf{d}_1 = g_i \mathbf{d}_1$ for orientations $V(\mathbf{a}_i', \mathbf{b}_i')$.

The set of the conjugate scanning groups $\mathcal{H}_i$ is obtained from the coset resolution of the space group, which corresponds to the coset resolution (5.2.2.2) of the point group:

$$\mathcal{G} = \mathcal{H}_1 \cup \{g_2|\mathbf{s}_2\}\mathcal{H}_1 \cup \ldots \cup \{g_p|\mathbf{s}_p\}\mathcal{H}_1. \qquad (5.2.2.3)$$

The scanning groups $\mathcal{H}_i = \{g_i|\mathbf{s}_i\}\mathcal{H}_1\{g_i^{-1}| - g_i^{-1}\mathbf{s}_i\}$ are related in the same way to the respective conventional bases $(\mathbf{a}_i', \mathbf{b}_i', \mathbf{d}_i) = (g_i\mathbf{a}_1', g_i\mathbf{b}_1', g_i\mathbf{d}_1)$ and hence they are expressed by the same Hermann–Mauguin symbols. However, the operations in the three-dimensional Euclidean space, which correspond to operations g_i on the vector space, often contain additional translations $\mathbf{s}_i$. Quite generally, the scanning for an orientation $V(\mathbf{a}_i', \mathbf{b}_i')$ is described in the same manner with reference to the coordinate system $(P + \mathbf{s}_i; V(\mathbf{a}_i', \mathbf{b}_i', \mathbf{d}_i))$ as the scanning for the orientation $V(\mathbf{a}_1', \mathbf{b}_1')$ is described with reference to a coordinate system $(P; V(\mathbf{a}_1', \mathbf{b}_1', \mathbf{d}_1))$.

In analogy with Wyckoff positions, see Section 8.3.2 of *IT* A, we distinguish three types of orientations and of orientation orbits:

(1) *special orientations and special orientation orbits with fixed parameters*;

(2) *special orientations and special orientation orbits with variable parameter*; and

(3) *general orientations and general orientation orbits*.

The type of the orbit is the same as the type of each of its orientations. Orientations and orientation orbits have the following characteristic properties:

(1) An orientation $V(\mathbf{a}', \mathbf{b}')$ is a *special orientation with fixed parameters* if its symmetry H is either at least orthorhombic or if it is monoclinic with the vector of its unique axis orthogonal to the orientation.

(2) An orientation $V(\mathbf{a}', \mathbf{b}')$ is a *special orientation with variable parameter* if its symmetry H is monoclinic and if it contains the vector of the unique axis.

(3) An orientation $V(\mathbf{a}', \mathbf{b}')$ is a *general orientation* if its symmetry H is triclinic.

Example 1

Orientations defined by the Miller indices (001) are special orientations with fixed parameters for monoclinic groups with unique axis c as well as for orthorhombic and tetragonal groups. Bravais–Miller indices (0001) also define special orientation with fixed parameters. In each of these cases, the orientation orbit contains just one orientation.

Orientations (010) and (100) are special orientations with fixed parameters for all orthorhombic groups and each such orientation constitutes the orientation orbit.

Orientations (001), (010) and (100) are special orientations with fixed parameters for cubic groups and they belong to the same orientation orbit.

Example 2

Orientations (*mn*0) are special orientations with variable parameter for monoclinic groups with unique axis *c*. Each such orientation constitutes an orientation orbit.

For cubic groups, the orientations (*mn*0) [with the exclusion of cases $m = \pm 1$, $n = 0$ and $m = 0$, $n = \pm 1$ in groups of Laue class $m\bar{3}$ (T_h) and also of cases $m = \pm 1$, $n = \pm 1$ in groups of Laue class $m\bar{3}m$ (O_h)] are special orientations with variable parameter. The orientation orbits contain six equivalent orientations in groups of Laue class $m\bar{3}$ (T_h) and 12 in groups of Laue class $m\bar{3}m$ (O_h), see Section 5.2.4.6.

Orientation orbits are correlated with orbits of crystal faces, see Part 10 of *IT* A. If the group H does not contain elements that change the sign of the normal, then the orientation orbit is characterized by the same set of Miller indices as the set of equivalent crystal faces. Generally, the group H contains a halving subgroup H_o whose elements leave the normal to the orientation $V(\mathbf{a}', \mathbf{b}')$ invariant while elements of the coset change its sign. In this case, the number of equivalent crystal faces is twice the number of orientations in the orbit. The group H_o is identical with the point symmetry of a crystal face of orientation $V(\mathbf{a}', \mathbf{b}')$. Such a face located at a point $P + s\mathbf{d}$ is sent to a face of the same orientation located at a point $P - s\mathbf{d}$ by those elements of H which are not contained in H_o. These are the same elements which change the direction of the scanning.

5.2.2.6. Linear orbits

We consider a section plane with orientation $V(\mathbf{a}', \mathbf{b}')$ and location $P + s\mathbf{d}$. The orbit of planes generated by the action of the scanned group $\mathcal{G}$ on this section plane splits into subsets of planes with the same orientation. The suborbit of planes with the same orientation is identical with the orbit under the action of the scanning group for this orientation. This suborbit is called the *linear orbit* of planes. If the orientation orbit contains only one orientation (scanning group = scanned group), then the linear orbit contains all planes of the orbit. If there are several orientations in the orientation orbit, then to each of these orientations there corresponds its own linear orbit. As shown in the previous section, the description of the scanning with reference to corresponding coordinate systems is identical for different orientations of the orientation orbit. The separation of planes and their sectional layer symmetries are the same in each of these orbits. In other words, the spatial distribution of layer symmetries is the same for all orientations of the orientation orbit; the scanning, however, begins generally at a point $P + \mathbf{s}_i$ for the orientation

$V(\mathbf{a}_i', \mathbf{b}_i')$. We shall concentrate our attention now to one linear orbit.

The parameter s in the description of linear orbits defines the position of the section plane by its intersection $P + s\mathbf{d}$ with the scanning line. The parameter therefore specifies the distance of the section plane from the origin P in units of $\mathbf{d}$ and is referred to as the *level* at which the section plane is located. Intersections at $P + (s + n)\mathbf{d}$, $n \in Z$ (integer) are translationally equivalent to an intersection at $P + s\mathbf{d}$ where $0 \leq s < 1$. The section planes at levels $P + (s + n)\mathbf{d}$ form an orbit under the translation group $T(\mathbf{d})$ generated by the scanning vector $\mathbf{d}$. The set of these planes is called the *translation orbit*. Each translation orbit has exactly one representative plane in the interval $0 \leq s < 1$. The linear orbit consists of one or several translation orbits.

We distinguish two types of locations and linear orbits:

(1) *Special locations of section planes and special linear orbits.*

(2) *General locations of section planes and general linear orbits.*

With reference to parameter s, the special locations always correspond to a fixed parameter, the general locations to a variable parameter. Special locations are singular in the sense that in the infinitesimal vicinity of a section plane at a special location there are only section planes of general location. The sectional layer groups corresponding to these locations have the following properties:

(1) The sectional symmetry of a plane in a special location is a layer group which contains operations changing the direction of the normal to the plane.

(2) The sectional symmetry of a plane in a general location is a layer group which does not contain operations changing the direction of the normal to the plane.

(3) The sectional symmetries of planes in special locations are always maximal layer subgroups of the space group $\mathcal{G}$ as well as of the scanning group $\mathcal{H}$. The sectional symmetry of a plane in a general location is a common halving subgroup of all sectional layer groups for special locations. We say that such a sectional layer group is *floating* in the scanning direction.

Comment: If the point group H of the scanning group $\mathcal{H}$ does not contain elements that change the normal to section planes, then all locations are general locations and there is only one sectional layer group common to all locations of section planes. The scanning group with this property is also called floating in the scanning direction.

The number of planes in a translation orbit: The total number of planes in a translation orbit is infinite because the index of the sectional layer group in the scanning group is. We can, however, count the number of planes in a translation orbit in an interval $0 \leq s < 1$. If the point group of the scanning group is H and the point group of the sectional layer group for a given translation orbit is L, then the number of planes in this orbit in the interval $0 \leq s < 1$ equals the index $[H : L]$ when the centring of the scanning group is P or C. When the centring of the scanning group is A, B, I or F, this number is $2[H : L]$; when the centring type of the scanning group is R, this number is $3[H : L]$.

The number f of planes in an orbit with a general parameter s per unit interval also defines the length of the fundamental region of the space group $\mathcal{G}$ as well as of the scanning group $\mathcal{H}$ in this interval. This length s_o is a fraction of unit interval, $s_o = \frac{1}{f}$, where $f = [H : L]$, $2[H : L]$ or $3[H : L]$ according to the centring of the scanning group and L is the point group of sectional layer groups corresponding to a general orbit.

5.2.2.7. Orthogonal, inclined and triclinic scanning

It is convenient for future reference to refine the basic categories of orthogonal and inclined scanning as follows:

(1) *Orthogonal scanning*. We call the scanning orthogonal if the scanning group is orthorhombic, tetragonal, trigonal or hexagonal.

(2*a*) *Monoclinic/orthogonal scanning*. This term is used if the scanning group is monoclinic and the vector $\mathbf{d}$ defines its unique axis.

In both cases the vector $\mathbf{d}$ is orthogonal to the vectors $\mathbf{a}'$ and $\mathbf{b}'$ and they occur whenever the orientation orbit is a special orbit with fixed parameters.

The absolute value $d = |\mathbf{d}|$ of the scanning vector is, in cases of orthogonal scanning, equal to the interplanar distance defined by the Miller indices of the orientation.

(2*b*) *Monoclinic/inclined scanning*. The scanning is called monoclinic/inclined if the scanning group is monoclinic and its unique axis is one of the vectors $\mathbf{a}'$, $\mathbf{b}'$. The vector $\mathbf{d}$ is actually not necessarily inclined to the orientation $V(\mathbf{a}', \mathbf{b}')$. It may be orthogonal owing to special metric conditions of the lattice which are determined by the scanned group $\mathcal{G}$. It is, however, a vector of a monoclinic basis which lies in the plane orthogonal to the unique axis. This case occurs when the orientation orbit is a special orbit with one variable parameter.

The interplanar distance d in the case of inclined scanning is $d = |\mathbf{d}| \cos\varphi$ where φ is the angle of the vector $\mathbf{d}$ with the normal to the plane.

(3) *Triclinic scanning*. The scanning is called triclinic or trivial if the scanning group is triclinic. This case occurs when the orientation orbit is a general orbit.

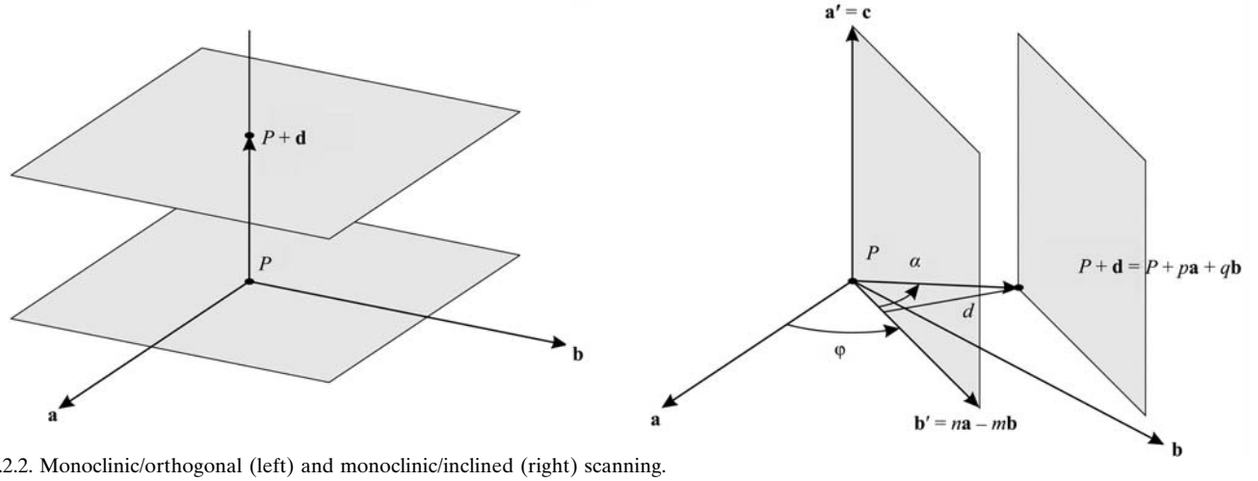

Fig. 5.2.2.2. Monoclinic/orthogonal (left) and monoclinic/inclined (right) scanning.

The difference between monoclinic/orthogonal and monoclinic/inclined scanning is illustrated in Fig. 5.2.2.2. The orientation in the first case is fixed, while the second case applies to various orientations containing the monoclinic unique axis. The orientation can be defined by one free parameter, the angle φ; we use instead Miller indices ($mn0$).

5.2.3. The contents and arrangement of the scanning tables

In the scanning tables two formats are used:

Standard format: This is the format in which the complete tables for triclinic and monoclinic groups and the tables of orthogonal scanning for all other groups are presented.

Auxiliary tables: These tables represent, in an abbreviated form, the cases where the scanned group is orthorhombic or belongs to a higher system and the orientation defines monoclinic/inclined scanning. The scanning is represented implicitly by referring to respective tables of monoclinic groups. [Note that in the online version of this volume the auxiliary tables are supplemented by explicit scanning tables.]

The tables are grouped according to crystallographic systems. Within each system, the standard-format tables are grouped into geometric classes in the same order as in *IT* A. The auxiliary tables follow the tables of standard format at the end of each Laue class.

5.2.3.1. The standard format

The content and arrangement of the standard-format tables are as follows:

(1) Headline.
(2) Orientation orbit.
(3) Conventional basis of the scanning group.
(4) Scanning group.
(5) Translation orbit.
(6) Sectional layer group.

The standard tables for triclinic groups describe the trivial scanning where the scanning group is $P1$ or $P\bar{1}$. The tables for monoclinic groups describe monoclinic/orthogonal scanning and monoclinic/inclined scanning. The standard tables for the remaining groups describe only orthogonal scanning for these groups.

5.2.3.1.1. Headline

The headline begins with the serial number of the space-group type identical with the numbering given in *IT* A, followed by a short Hermann–Mauguin symbol. The Schönflies symbol is given in the upper right-hand corner.

The next line is centred and contains the full Hermann–Mauguin symbol of the specific space group for which the scanning is described in the table. This is followed by a statement of origin in those cases where two space groups of different origin are considered, or by a statement of cell choice when different cell choices are used for a monoclinic space group.

The specific space group considered in the table is that space group, including its orientation (setting) and location (origin choice), the diagram of which is presented in *IT* A, assuming that the upper left-hand corner of the diagram represents the origin P, its left edge downwards the vector **a**, its upper edge to the right the vector **b**, while vector **c** is directed upwards. In the case of orthorhombic and monoclinic groups, this is the diagram in the (abc) setting, the so-called standard setting. For some group types, two different origins are given in *IT* A. Both are used to consider two specific groups of the same type with different locations in the present tables. The scanning for each of these groups is described in a separate table. In the case of monoclinic groups, one, three or six different cell choices, depending on the group type, are considered, see Section 5.2.4.2.

5.2.3.1.2. Orientation orbit

Each table is divided into five columns. The first column is entitled *Orientation orbit* (hkl) or *Orientation orbit* ($hkil$). The orientations are specified by their Miller or Bravais–Miller indices. Each orientation defines a row for which the scanning is described in the next columns. Orientations which belong to the same orbit are grouped together and orientation orbits are separated by horizontal double lines across the table for space groups of the tetragonal and higher-symmetry systems and for the monoclinic groups. The vertical separation for orthorhombic groups is explained in Section 5.2.4.3.

Orientation orbits are listed in each table in the following order from top to bottom:

(1) Special orientation orbits with fixed parameters which contain just one orientation. Such orbits do not occur in triclinic and cubic groups.

(2) Special orientation orbits with fixed parameters which contain several orientations. Such orbits do not occur in triclinic, monoclinic and orthorhombic groups.

(3) Special orientation orbits with variable parameter. Such orbits do not occur in triclinic groups. They are presented in standard format for monoclinic groups. In this case, the orientations are defined by Miller indices ($n0m$) (unique axis b) or ($mn0$) (unique axis c) and the orbit contains just one orientation. For higher symmetries, these orbits contain several orientations which are given in the auxiliary tables.

General orientation orbits are not included; the corresponding scanning is trivial and the presentation of these orbits would take up too much space.

5.2.3.1.3. The scanning group and its conventional basis

The second column is entitled *Conventional basis of the scanning group* and it contains three subcolumns headed by the symbols of vectors $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{d}$. Next to it is the third column with the heading *Scanning group* $\mathcal{H}$. In the subcolumns, the vectors $\mathbf{a}'$, $\mathbf{b}'$ and $\mathbf{d}$ of the conventional bases of the scanning groups $\mathcal{H}$ are specified in terms of the conventional basis (**a**, **b**, **c**) of the scanned group $\mathcal{G}$. The scanning groups are described in the third column by their short Hermann–Mauguin symbols.

(1) *Orbits with one orientation*: With the exception of cubic groups, all space groups are reducible so that the orientations (001) or (0001) are invariant under the point group G and the orbit contains only one orientation. The scanning group $\mathcal{H}$ in these cases is identical with the scanned group $\mathcal{G}$ and its conventional basis ($\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{d}$) is identical with the conventional basis (**a**, **b**, **c**) so that the groups $\mathcal{G}$ and $\mathcal{H}$ are denoted by the same Hermann–Mauguin symbol. The row for this orientation is always listed first.

The scanning group $\mathcal{H}$ also coincides with the scanned group $\mathcal{G}$ for the orientations (100) and (010) in orthorhombic groups. However, the Hermann–Mauguin symbol for the scanning group may differ from that of the scanned group. This is a result of having the $\mathbf{a}'$ and $\mathbf{b}'$ basis vectors of the scanning group always representing the basis vectors of the resulting sectional layer