International Tables for Crystallography (2006). Vol. E, Chapter 5.2, pp. 393–416.

5.2. Guide to the use of the scanning tables

5.2.1. Introduction

The global symmetry of an ideal crystal is described by its space group $\mathcal{G}$. It is also of interest to consider symmetries of local character. The classical example is that of the site symmetries, which are the symmetries of individual points in a crystal. These are completely described and classified as a part of the standard description of space groups in *International Tables for Crystallography*, Volume A, *Space-Group Symmetry* (*IT* A, 1983). The results of this procedure contain two types of information:

(i) site symmetries of individual points under the action of the group $\mathcal{G}$ and

(ii) orbits of points under the action of the group $\mathcal{G}$.

This information, apart from its use, for example, in the consideration of the splitting of atomic levels in the field of the site symmetry, provides the background for the description of crystal structure: points of the same orbit are occupied by identical atoms (ions) and the environment of these atoms (ions) is also identical. A complete description of the structure is reduced to a description of the occupation of individual Wyckoff positions.

Analogously, we may consider the symmetries of planes transecting the crystal and of straight lines penetrating the crystal, called here the *sectional layer groups* (*symmetries*) and the *penetration rod groups* (*symmetries*). Here we look again for the two types of information:

(i) symmetries of individual planes (straight lines) under the action of the group $\mathcal{G}$ and

(ii) orbits of planes (straight lines) under the action of the group $\mathcal{G}$.

The general law that describes the connection between local symmetries and orbits of points, planes or straight lines is expressed by a coset resolution of the space group with respect to local symmetries. The orbits of planes (straight lines) have analogous properties to orbits of points. The structure of the plane (straight line) and its environment is identical for different planes (straight lines) of the same orbit. This is useful in the consideration of layer structures, see Section 5.2.5.1, and of structures with pronounced rod arrangements.

Layer symmetries have also been found to be indispensable in *bicrystallography*, see Section 5.2.5.2. This term and the term *bicrystal* were introduced by Pond & Bollmann (1979) with reference to the study of grain boundaries [see also Pond & Vlachavas (1983) and Vlachavas (1985)]. A bicrystal is in general an edifice where two crystals, usually of the same structure but of different orientations, meet at a common boundary – an interface. The sectional layer groups are appropriate for both the description of symmetries of such boundary planes and the description of the bicrystals.

The *sectional layer groups* were, however, introduced much earlier by Holser (1958*a*,*b*) in connection with the consideration of domain walls and twin boundaries as symmetry groups of planes bisecting the crystal. The mutual orientations of the two components of a bicrystal are in general arbitrary. In the case of domain walls and twin boundaries, which can be considered as interfaces of special types of bicrystals, there are crystallographic restrictions on these orientations. The group-theoretical basis for an analysis of domain pairs is given by Janovec (1972). The consideration of the structure of domain walls or twin boundaries involves the sectional layer groups (Janovec, 1981; Zikmund, 1984); they were examined in the particular cases of domain structure in KSCN crystals (Janovec *et al.*, 1989) and of domain walls and antiphase boundaries in calomel crystals (Janovec & Zikmund, 1993), see Section 5.2.5.3, and recently also in fullerene C_{60} (Janovec & Kopský, 1997; Saint-Grégoire, Janovec & Kopský, 1997).

The first attempts to derive the sectional layer groups systematically were made by Wondratschek (1971) and by using a computer program written by Guigas (1971). Davies & Dirl (1993*a*) developed a program for finding subgroups of space groups, which they later modified to find sectional layer groups and penetration rod groups as well (Davies & Dirl, 1993*b*). The use and determination of sectional layer groups have also been discussed by Janovec *et al.* (1988), Kopský & Litvin (1989) and Fuksa *et al.* (1993).

The penetration rod groups can be used in the consideration of linear edifices in a crystal, *e.g.* line dislocations or intersections of boundaries, or in crystals with pronounced rod arrangements. So far, there seems to be no interest in the penetration rod groups and there is actually no need to produce special tables for these groups. Determining penetration rod groups was found to be a complementary problem to that of determining sectional layer groups (Kopský, 1989*c*, 1990).

The keyword for this part of this volume is the term *scanning*, introduced by Kopský (1990) for the description of the spatial distribution of local symmetries. In this sense, the description of site symmetries and classification of point orbits by Wyckoff positions are a result of the *scanning* of the space group for the site symmetries.

The *Scanning tables*, Part 6, give a complete set of information on the space distribution of sectional layer groups and of the penetration rod groups. They were derived using the *scanning-group* method and the *scanning theorem*, see Section 5.2.2.2. The tables describe explicitly the scanning for the sectional layer groups. The spatial distribution of (scanning for) the penetration rod groups is seen directly from the *scanning groups*, which are given as a part of the information in the scanning tables.

The sectional layer groups and the penetration rod groups are subgroups of space groups and as such act on the three-dimensional point space. The examples of particular studies in Section 5.2.5 emphasize the importance of the exact location of sectional layer groups with reference to the crystal structure and hence to the crystallographic coordinate system. In the usual interpretation, Hermann–Mauguin symbols do not specify the location of the group in space. In the scanning tables, each Hermann–Mauguin symbol means a quite specific space or layer group with reference to a specified crystallographic coordinate system, see Sections 5.2.3.1.1 and 5.2.3.1.4.

The layer and rod groups can also be interpreted as factor groups of reducible space groups (Kopský, 1986, 1988, 1989*a*,*b*, 1993*a*; Fuksa & Kopský, 1993). Our choice of standard Hermann–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.

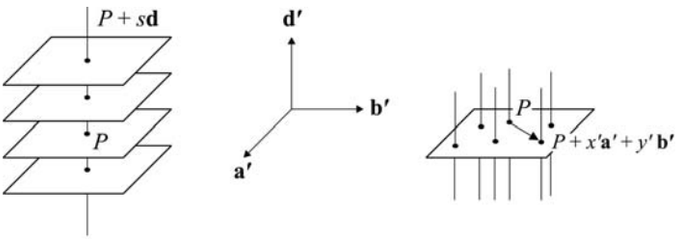

Fig. 5.2.2.1. Sets of parallel planes (left) and sets of parallel straight lines (right).

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 $\mathbf{a}'$, $\mathbf{b}'$.

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 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

[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.

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

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

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 Part 9 [page 735, (vi) and (vii)] of *IT* A (1983).

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.

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

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

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 ($mn0$) 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 ($mn0$) [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 **d** defines its unique axis.

In both cases the vector **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 **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 **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.

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 (*mn*0).

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.

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

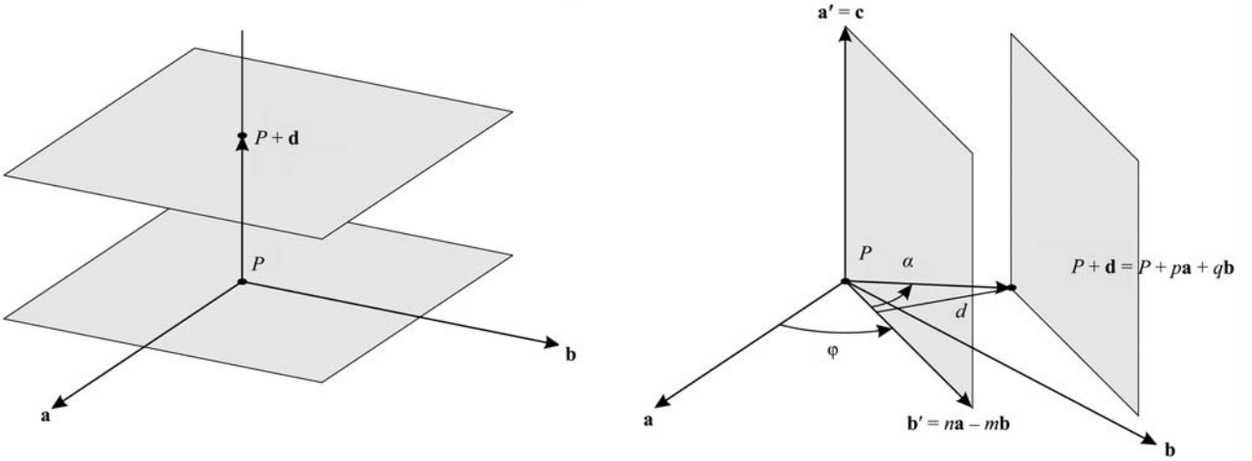

Fig. 5.2.2.2. Monoclinic/orthogonal (left) and monoclinic/inclined (right) scanning.

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 (*n*0*m*) (unique axis *b*) or (*mn*0) (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 ($\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$) 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 ($\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$) 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 groups. The alternative setting symbols used are those listed in Table 4.3.1 of Part 4 of *IT* A.

Example: Space group *Pbcn*, D_{2h}^{14} (No. 60). The group itself is the scanning group for all three orientations (001), (100) and (010). However, in view of the conventional choice of the basis of the scanning group, its symbols are *Pbcn*, *Pbna* and *Pnca*, respectively.

Monoclinic groups. The scanning group $\mathcal{H}$ coincides with the scanned group $\mathcal{G}$ for the orientations (010) (unique axis *b*) and (001) (unique axis *c*). These are the cases of monoclinic/orthogonal scanning and, according to convention, the scanning vector $\mathbf{d}$ is chosen as the vector of the unique axis. The symbol of the scanning group coincides with the Hermann–Mauguin symbol for unique axis *c* in both cases.

The scanning group $\mathcal{H}$ also coincides with the scanned group $\mathcal{G}$ for orientations (*n*0*m*) (unique axis *b*) or (*mn*0) (unique axis *c*). These cases lead to monoclinic/inclined scanning described below in conjunction with the auxiliary tables. Vector $\mathbf{a}'$ is, in these cases, chosen as the vector of the unique axis. Since this vector is considered as the first vector in the conventional basis of the scanning group, the Hermann–Mauguin symbols for the scanning group are the symbols that correspond to unique axis *a*. They may differ further depending on the choice of vectors $\mathbf{b}'$ and $\mathbf{d}$.

(2) *Orbits with several orientations*: There are several Miller indices in each box of the first column which denote the orientations belonging to one orientation orbit. In the three subcolumns of the second column, the conventional bases of the scanning groups $\mathcal{H}_i$, *i.e.* the vectors $\mathbf{a}_i'$, $\mathbf{b}_i'$, $\mathbf{d}_i$, are specified in terms of the conventional basis vectors $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ of the space group $\mathcal{G}$ and of the Miller indices. The vectors $\mathbf{a}_i'$, $\mathbf{b}_i'$, $\mathbf{d}_i$ then represent the conventional bases with respect to which the scanning groups $\mathcal{H}_i$ are given by their Hermann–Mauguin symbols in the third column. These scanning groups are of the same type for all orientations of the orbit and they are also oriented in the same way with respect to their bases; they may, however, have different origins. Therefore, the Hermann–Mauguin symbols of the scanning groups are the same for all orientations of a given orbit up to a possible shift of origin.

Example: Space groups $P42_12$, D_4^2 (No. 90), $P4_122$, D_4^3 (No. 91) and $P4_12_12$, D_4^4 (No. 92), the orientation orbit (100) and (010): In the case of the group $P42_12$, the scanning groups for the orientations (100) and (010) are denoted by the same symbol $P2_122_1$ with reference to coordinate systems $(P; \mathbf{a}', \mathbf{b}', \mathbf{d}) = (P; \mathbf{b}, \mathbf{c}, \mathbf{a})$ and $(P; \mathbf{a}', \mathbf{b}', \mathbf{d}) = (P; -\mathbf{a}, \mathbf{c}, \mathbf{b})$, respectively.

In the case of the group $P4_122$, the scanning group for the orientation (100) is written as $P22_12$ ($\mathbf{b}'/4$). This is equivalent to the statement that the scanning group is the group $P22_12$ with reference to coordinate system $(P + \mathbf{b}'/4; \mathbf{a}', \mathbf{b}', \mathbf{d}) = (P + \mathbf{c}/4; \mathbf{b}, \mathbf{c}, \mathbf{a})$. The scanning group for the orientation (010) is the group $P22_12$ with reference to coordinate system $(P; \mathbf{a}', \mathbf{b}', \mathbf{d}) = (P; -\mathbf{a}, \mathbf{c}, \mathbf{b})$.

In the case of the group $P4_12_12$, we conclude analogously that the scanning group for the orientation (100) is the group $P2_12_12_1$ with reference to coordinate system $(P + 3\mathbf{b}'/8 + \mathbf{d}/4; \mathbf{a}', \mathbf{b}', \mathbf{d}) = (P + 3\mathbf{c}/8 + \mathbf{a}/4; \mathbf{b}, \mathbf{c}, \mathbf{a})$, while for the orientation (010) it is the group $P2_12_12_1$ with reference to coordinate system $(P + \mathbf{b}'/8 + \mathbf{d}/4; \mathbf{a}', \mathbf{b}', \mathbf{d}) = (P + \mathbf{c}/8 + \mathbf{b}/4; -\mathbf{a}, \mathbf{c}, \mathbf{b})$.

The vectors $\mathbf{a}_i'$, $\mathbf{b}_i'$ also define the translation subgroup T_{Gi} of all sectional layer groups corresponding to a given orientation, which are listed in the fifth column. The vectors either themselves constitute the conventional basis of these layer groups or the conventional basis is expressed through them.

The scanning groups $\mathcal{H}_i$ are conjugate subgroups of the space group $\mathcal{G}$ in cases when there is more than one orientation in the orbit. They are accordingly expressed by the same Hermann–Mauguin symbol with respect to different coordinate systems. There are cases when the origins of these coordinate systems for the conjugate scanning groups $\mathcal{H}_i$ coincide. In this case, one block of the table is sufficient to describe the scanning groups, the translation orbits and the corresponding sectional layer groups in the same manner as in the case of an orbit with one orientation. The common origin $P + \boldsymbol{\tau}$ is stated in a line above the block in the form 'With respect to origin at $P + \boldsymbol{\tau}$' if it is different from the origin P of the coordinate system of the scanned group $\mathcal{G}$.

When origins are different, there appear several blocks with Hermann–Mauguin symbols of the scanning group at different locations for different orientations. The blocks are then separated

by horizontal lines through the last three columns. Two ways are used to express the fact that the origin of the scanning group does not coincide with the origin of the original group $\mathcal{G}$. We use the Hermann–Mauguin symbol of the scanning group with the statement of the shift of its origin (as a rule below the symbol) for each of the separated blocks. In some cases, for typographical reasons, we state with respect to which origin the Hermann–Mauguin symbol of the scanning group, and consequently the description of the translation orbit and of the sectional layer groups, is referring to.

5.2.3.1.4. *The linear orbits and sectional layer groups*

The fourth column, headed *Linear orbit* $s\mathbf{d}$, describes the linear orbits of planes for the orientation of this row and the fifth column, headed *Sectional layer group* $\mathcal{L}(s\mathbf{d})$, describes the corresponding sectional layer groups.

The location of the plane along the line $P + s\mathbf{d}$ determines a certain layer group; the symbol $\mathcal{L}(s\mathbf{d})$ next to $s\mathbf{d}$ is a shorthand for the sectional layer group $\mathcal{L}(P + s\mathbf{d}, (hkl))$ of the section plane passing through the point $P + s\mathbf{d}$ on the scanning line. $\mathcal{L}(s\mathbf{d})$, as a function of s, has a periodicity of the translation normalizer of the space group $\mathcal{G}$ in the direction $\mathbf{d}$ but we list the translation orbits within $0 \leq s < 1$, *i.e.* with periodicity $\mathbf{d}$. This is important because the planes at levels separated by the periodicity of the normalizer do not necessarily belong to the same orbit.

The planes form orbits with fixed parameter s and with a variable parameter s. The orbits with fixed parameter s are recorded in terms of fractions of vector $\mathbf{d}$; one of these fractions always lies in the interval $0 \leq s < s_o$, where s_o is the length of the fundamental region of the scanned group $\mathcal{G}$ along the scanning line $P + s\mathbf{d}$ in units of $\mathbf{d}$. The fixed values of s are always given in the range $0 \leq s < 1$. If planes at different levels belong to the same orbit, then the levels are enclosed in square brackets. The sectional layer group corresponding to a certain level s is then given in the fifth column by its Hermann–Mauguin symbol in the coordinate system $(P + s\mathbf{d}; \mathbf{a}', \mathbf{b}', \mathbf{d})$. If the levels on the same line refer to the same Hermann–Mauguin symbol of a sectional layer group but are not enclosed in brackets, then they belong to different orbits. The sectional layer groups belonging to different planes of the orbit are certainly of the same type and parameters but they may be oriented or located in different ways so that their Hermann–Mauguin symbols are different because they refer to the same basis $(\mathbf{a}', \mathbf{b}')$. In this case, the levels corresponding to the same orbit are listed in a column, beginning and ending with brackets, and to each level is given the sectional layer group.

There is always only one row (which may, however, split for typographical reasons) corresponding to orbits with a variable parameter s and the one sectional layer group which is floating along the scanning direction and which is a common subgroup of all sectional layer groups for orbits with fixed parameters. This row always contains the term $s\mathbf{d}$ where s belongs to the fundamental region $0 \leq s < s_o = \frac{1}{f}$ of the group $\mathcal{G}$ along the line $P + s\mathbf{d}$. Here s_o is a fraction of 1 and the region is a fraction of the interval $0 \leq s < 1$. These levels correspond to locations of planes of the translation orbit along the direction $\mathbf{d}$ within the unit interval. The levels are expressed in a compact way; as a result there appears an entry $\pm s\mathbf{d}$ in cases when the scanning group is not polar. Since s is in the interval $0 \leq s < s_o$, $-s$ is negative and hence not in the interval $0 \leq s_i < 1$; this level is equivalent to the level $(1 - s)\mathbf{d}$.

Following each Hermann–Mauguin symbol, we give the sequential number of the type to which the sectional layer group belongs, according to its numbering in Parts 1–4 of this volume.

Example 1: Orientation orbit (001) for the space groups $P422$, D_4^1 (No. 89), $P4_222$, D_4^5 (No. 93) and $P4_122$, D_4^3 (No. 91).

Group $P422$: The entries '$0\mathbf{d}, \frac{1}{2}\mathbf{d}$' in the fourth column followed by $p422$ in the fifth column indicate that there are two separate translation orbits, represented by planes passing through P and $P + \frac{1}{2}\mathbf{d}$; planes of both orbits have the same sectional layer group with reference to the respective coordinate systems.

The sectional layer symmetry at a general level is $p4$ and the translation orbit contains planes at two levels (the index of the point group 4 in the point group 422), described as $[s\mathbf{d}, -s\mathbf{d}]$. It is $s_o = \frac{1}{2}$ and both levels $\pm s\mathbf{d}$ belong to the same orbit. For positive s we can change $-s$ to $(1 - s)$ to get the level in the interval $0 \leq s_i < 1$.

Group $P4_222$: The entries $[0\mathbf{d}, \frac{1}{2}\mathbf{d}]$ are now enclosed between square brackets to indicate that the planes at these levels along the line $P + s\mathbf{d}$ belong to the same orbit. The sectional layer symmetry is $p222$.

The sectional layer symmetry at a general level is $p112$, so that there must be four [422 (D_4) : 122 (C_2)] levels which are described as $[\pm s\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}]$ where $0 < s < s_o = \frac{1}{4}$. Again we can change $-s$ to $(1 - s)$ to get the level in the interval $0 < s_i < 1$.

Group $P4_122$: The entry '$[0\mathbf{d}, \frac{1}{2}\mathbf{d}$;' in the first subrow and the entry '$\frac{1}{4}\mathbf{d}, \frac{3}{4}\mathbf{d}]$' in the second subrow indicate that the planes on corresponding levels all belong to the same translation orbit. The corresponding sectional layer groups $p121$ and $p211$ for the first and second subrow are of the same type but the orientations of their twofold axes are different. The Hermann–Mauguin symbols are therefore different because they are expressed with reference to the same basis [in this case the basis $(\mathbf{a}, \mathbf{b})$].

The sectional layer symmetry at a general level is $p1$ so that $s_o = \frac{1}{8}$ and there must be eight levels which are described as $[\pm s\mathbf{d}, (\pm s + \frac{1}{4})\mathbf{d}, (\pm s + \frac{1}{2})\mathbf{d}, (\pm s + \frac{3}{4})\mathbf{d}]$.

Example 2: We consider the group $R\bar{3}$, C_{3i}^2 (No. 148) and the orientation (0001). There are three subrows in the columns for the translation orbits and the sectional layer groups. In the first row there are the entries $[0\mathbf{d}, [\frac{1}{2}\mathbf{d}$; and $p\bar{3}$; in the second row $\frac{1}{3}\mathbf{d}$, $\| \frac{5}{6}\mathbf{d}$, and $p\bar{3}$ $[(2\mathbf{a} + \mathbf{b})/3]$; and in the third row $\frac{2}{3}\mathbf{d}] \frac{1}{6}\mathbf{d}]$ and $p\bar{3}$ $[(\mathbf{a} + 2\mathbf{b})/3]$. This is to be interpreted as follows: the levels $[0\mathbf{d}, \frac{1}{3}\mathbf{d}$ and $\frac{2}{3}\mathbf{d}]$ belong to one translation orbit, distinct from the orbit to which belong the levels $[\frac{1}{2}\mathbf{d}, \frac{5}{6}\mathbf{d}$ and $\frac{1}{6}\mathbf{d}]$. The sectional layer groups are groups $p\bar{3}$ on all these levels but they are located at different distances from points $P + s\mathbf{d}$ for different levels $s\mathbf{d}$.

The sectional layer symmetry at a general level is $p3$. The point group 3 is of index 2 in the point group $\bar{3}$ and the lattice is of the type R so there are six planes in the translation orbit per unit interval along $\mathbf{d}$ and $s_o = \frac{1}{6}$. The translation orbit is described by $[\pm s\mathbf{d}, (\pm s + \frac{1}{3})\mathbf{d}, (\pm s + \frac{2}{3})\mathbf{d}]$.

Example 3: Space group $P4/mmm$, D_{4h}^1 (No. 123). The scanning groups for the orientations (100) and (010) which belong to the same orientation orbit are expressed by the same Hermann–Mauguin symbol *Pmmm* in their respective bases. The translation orbits and sectional layer groups are therefore expressed in the same block.

The scanning groups for the orientations (110) and $(1\bar{1}0)$ of the same orientation orbit under the space group $P4/nbm$, D_{4h}^3 (No. 125) are expressed by the same Hermann–Mauguin symbol *Bmcm* (**d**/4) in the respective bases if the scanned group is chosen according to origin choice 1 in *IT* A. Hence the translation orbits and sectional layer groups are expressed in one block; they are the same with reference to their corresponding bases. For origin choice 2, the locations of the scanning groups are different; we obtain the group *Bmcm* for the orientation (110) and *Bmcm* $[(\mathbf{a}' + \mathbf{d})/4]$ for the orientation $(1\bar{1}0)$. Each of these scanning groups has its own box with the translation orbits and sectional layer groups. If we compare the two boxes, we observe that the data in the second box are the same as in the first box but shifted by $[(\mathbf{a}' + \mathbf{d})/4]$.

Example 4: Consider the block of the orientation orbit (111), $(\bar{1}11)$, $(1\bar{1}1)$, $(11\bar{1})$ for space groups $P4_332$, O^6 (No. 212), $P4_132$, O^7 (No. 213) and $I4_132$, O^8 (No. 214). The Hermann–Mauguin symbol of the scanning group with reference to their bases is the

same, *R*32, up to a shift of the origin. In the row for each orientation, therefore not only are the bases given, but also the location of the origin so that a complete coordinate system is specified in such a way that the symbol is exactly the same for each orientation. The symbol of the scanning group, the location of the orbits and the sectional layer groups are given in the last block; all this information is formally the same but for each orientation it refers to its own coordinate system.

5.2.3.2. *Auxiliary tables*

The auxiliary tables describe cases of monoclinic/inclined scanning for groups of orthorhombic and higher symmetries. They are clustered together for groups of each Laue class, starting from Laue class D_{2h} – *mmm*, after the tables of orthogonal scanning, *i.e.* after the standard-format tables for this Laue class.

All possible cases of monoclinic/inclined scanning reduce to cases where the scanned group $\mathcal{G}$ itself is monoclinic and the orientation is defined by the Miller indices (*mn*0). These cases are described as a part of the standard-format tables for monoclinic groups. Two bases are used in this description:

(i) The conventional basis (**a**, **b**, **c**) of the group $\mathcal{G}$ in its role as the scanned group.

(ii) The conventional basis (in the sense of the convention for scanning groups, see Section 5.2.2.3) ($\mathbf{a}'$, $\mathbf{b}'$, **d**) of the group $\mathcal{H} = \mathcal{G}$ in its role as the scanning group.

If the scanned group $\mathcal{G}$ is of higher than monoclinic symmetry, then the monoclinic scanning group $\mathcal{H} \subset \mathcal{G}$ and we use three bases:

(i) The conventional basis (**a**, **b**, **c**) of the scanned group $\mathcal{G}$.

(ii) The conventional basis ($\widehat{\mathbf{a}}$, $\widehat{\mathbf{b}}$, $\widehat{\mathbf{c}}$) of the monoclinic scanning group $\mathcal{H}$, which is further called the *auxiliary basis*. This basis is always chosen so that the vector $\widehat{\mathbf{c}}$ is the unique axis vector.

(iii) The conventional basis (in the sense of the convention for scanning groups, see Section 5.2.2.3) ($\mathbf{a}'$, $\mathbf{b}'$, **d**) of the scanning group $\mathcal{H}$.

Two types of tables from which orbits of planes and sectional layer groups can be deduced are given:

(1) *Tables of orientation orbits and auxiliary bases of scanning groups*. These contain Miller indices of orientations in the orbit and define auxiliary bases ($\widehat{\mathbf{a}}$, $\widehat{\mathbf{b}}$, $\widehat{\mathbf{c}}$) of the respective scanning groups in terms of the basis (**a**, **b**, **c**) of the scanned group $\mathcal{G}$ and of the Miller indices of the orientation.

(2) *Reference tables*. These serve to give a reference to that table of a monoclinic group from which one can read the scanning data.

In the next two sections we describe the construction of these two types of tables and their use in detail.

5.2.3.2.1. *Tables of orientation orbits and auxiliary bases of scanning groups*

The cases of monoclinic/inclined scanning occur when the orientation of the section plane:

(i) contains the direction of some symmetry axis of even order [scanning group of geometric class 2 (C_2)],

(ii) is orthogonal to a symmetry plane [scanning group of geometric class *m* (C_s)],

(iii) contains the direction of some symmetry axis of even order and at the same time is orthogonal to a symmetry plane [scanning group of geometric class $2/m$ (C_{2h})].

Auxiliary basis of the scanning group. In each of these cases, there is a set of orientations for which the property (i), (ii) or (iii) is common and all orientations of this set contain the vector that defines the unique axis of a monoclinic scanning group which is also common for all orientations of the set. An auxiliary basis ($\widehat{\mathbf{a}}$, $\widehat{\mathbf{b}}$, $\widehat{\mathbf{c}}$) of this scanning group is defined with reference to that one orientation of the set which is described by Miller indices (*mn*0).

The first column of each table describes orientations of the orbit by Miller indices with reference to the conventional basis (**a**, **b**, **c**) of the scanned group $\mathcal{G}$. Various possible situations can be distinguished by three criteria:

(1) The structure of orbits.

(i) All orientations of the orbit contain the vector of the unique axis of the scanning group. This also means that there is only one scanning group for all orientations of the orbit.

This situation occurs for orientations that contain the vector of principal axis *c* in tetragonal and hexagonal groups. It occurs also for orientations which contain the vector of any of the orthorhombic axes *c*, *a* or *b*.

(ii) The orbit splits into sets of orientations where each set has its own common unique axis and scanning group.

This situation occurs for orientations that contain vectors of auxiliary axes of groups of Laue classes $4/mmm$ (D_{4h}), $\bar{3}m$ (D_{3d}), $6/mmm$ (D_{6h}), $m\bar{3}$ (T_h) and $m\bar{3}m$ (O_h).

(2) Possible increase of the symmetry for special orientations.

(i) All orientations of the set with common unique axis have the same monoclinic scanning group.

This is the case of groups of Laue classes $4/m$ (C_{4h}) and $6/m$ (C_{6h}), and of orientations that contain the vector **c** of the principal axis.

(ii) In all other cases there appear special orientations in the set which have higher symmetry than monoclinic.

(3) Auxiliary basis of the scanning group.

The auxiliary bases of scanning groups are their conventional bases corresponding to unique axis *c*.

(i) If the conventional basis of the scanning group can be based on the same vectors as the conventional basis of the scanned group, parameters *m*, *n* are used in the Miller indices that define the orientation.

(ii) If the conventional basis of the scanning group cannot be based on the same vectors as the conventional basis of the scanned group, parameters *h*, *k*, *l* are used in the Miller indices that define the orientation with reference to the conventional basis (**a**, **b**, **c**).

In these cases, the transformation of Miller indices with reference to the conventional basis (**a**, **b**, **c**) to Miller indices with reference to auxiliary basis ($\widehat{\mathbf{a}}$, $\widehat{\mathbf{b}}$, $\widehat{\mathbf{c}}$) is given in a row under the orientation orbit. The letters *m* and *n* are always used for Miller indices with reference to auxiliary bases.

The second column assigns to each orientation the conventional basis ($\mathbf{a}'$, $\mathbf{b}'$, **d**) of the monoclinic scanning group that is related to the auxiliary basis ($\widehat{\mathbf{a}}$, $\widehat{\mathbf{b}}$, $\widehat{\mathbf{c}}$) given in the third column in the same way as to the standard basis (**a**, **b**, **c**) in the case of monoclinic groups.

The conventional basis ($\mathbf{a}'$, $\mathbf{b}'$, **d**) is always chosen so that its first vector $\mathbf{a}'$ is the vector of the common unique axis. Vector $\mathbf{b}'$ is defined by the orientation of section planes and hence by Miller indices (either directly or indirectly through transformation to a monoclinic basis). There is the same freedom in the choice of the scanning direction **d** as in the cases of monoclinic/inclined scanning in the case of monoclinic groups.

5.2.3.2.2. *Reference tables*

Each table of orientation orbits for a certain centring type(s) is followed by reference tables which are organized by arithmetic classes belonging to this centring type(s). The scanned space groups $\mathcal{G}$ are given in the first row by their sequential number, Schönflies symbol and short Hermann–Mauguin symbol. They are arranged in order of their sequential numbers unless there is a clash with arithmetic classes; a preference is given to collect groups of the same arithmetic class in one table. If space allows it, groups of more than one arithmetic class are described in one table.

The first column is identical with the first column of the table of orientation orbits. On the intersection of a column which specifies the scanned group $\mathcal{G}$ and of a row which specifies the orientation by its Miller (Bravais–Miller) indices is found the scanning group, given by its Hermann–Mauguin symbol with reference to the auxiliary basis $(\widehat{\mathbf{a}}, \widehat{\mathbf{b}}, \widehat{\mathbf{c}})$. This symbol, which may also contain a shift of origin, instructs us which monoclinic scanning table to consult. The vectors $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{d}$ that determine the lattice of sectional layer groups and the scanning direction are those given in the table of orientation orbits. Depending on the values of parameters m, n, p, q we find the scanning group in its basis $(\mathbf{a}', \mathbf{b}', \mathbf{d})$ and the respective sectional layer groups.

5.2.4. Guidelines for individual systems

5.2.4.1. *Triclinic system*

The triclinic groups are trivial even from the viewpoint of scanning but it is non-trivial to express the vectors $\mathbf{a}'$, $\mathbf{b}'$ and $\mathbf{d}$ in terms of vectors $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ and of Miller indices (hkl). Since the groups are related in the same way with respect to any given basis, we do not identify bases in the two tables. The specification *Any admissible choice* for the scanning group means that the vectors $\mathbf{a}'$, $\mathbf{b}'$ have to be chosen as a basis of the translation group in the subspace defined by Miller indices and $\mathbf{d}$ should be the vector that completes the basis of the translation group in the whole space.

The scanned groups are identical with the scanning group for all orientations in the triclinic groups $P1$, C_1^1 (No. 1) and $P\bar{1}$, C_i^1 (No. 2). There is only one orientation in each orientation orbit. In the case of the group $P1$, C_1^1 (No. 1), there is one type of linear orbit consisting of planes generated by translations $\mathbf{d}$ from either one of the set and the respective layer symmetries are the trivial groups $p1$ (L01). In the case of the group $P\bar{1}$, C_i^1 (No. 2), the orbit with a general location consists of a pair of planes, located symmetrically from a symmetry centre at distances $\pm s$ in the scanning direction $\mathbf{d}$, which is then periodically repeated with periodicity $\mathbf{d}$; the sectional layer symmetry of these planes is $p1$ (L01). Furthermore, there are two linear orbits corresponding to positions $0\mathbf{d}$ and $\frac{1}{2}\mathbf{d}$, each of which consists of a periodic set of planes with periodicity $\mathbf{d}$; the sectional symmetry in each of these cases is $p\bar{1}$ (L02).

The triclinic scanning also applies to general orientation orbits of all space groups of higher symmetry than triclinic. If the space group $\mathcal{G}$ is noncentrosymmetric, then the number of orientations in the orientation orbit is the order $|G|$ of the point group G and the linear orbits are described for each orientation as in the case of the group $P1$, C_1^1 (No. 1). If the space group $\mathcal{G}$ is centrosymmetric, then the number of orientations in the orientation orbit is $|G|/2$ and the linear orbits are described for each orientation as in the case of the group $P\bar{1}$, C_i^1 (No. 2).

5.2.4.2. *Monoclinic system*

The scanning of monoclinic groups is non-trivial if the section planes are either orthogonal to or parallel with the unique axis. The first case results in monoclinic/orthogonal scanning, the second in monoclinic/inclined scanning.

Depending on the space-group type, a monoclinic group $\mathcal{G}$ admits one, three or six cell choices, which are illustrated and labelled by numbers 1, 2, 3 and $\tilde{1}$, $\tilde{2}$, $\tilde{3}$ in Fig. 5.2.4.1. For each cell choice, a separate table is given in which the group is specified by Hermann–Mauguin symbols with reference to unique axis b or to unique axis c.

Monoclinic/orthogonal scanning. There exists only one orientation orbit and it contains just one orientation. When the c axis is chosen as the unique axis, the scanning group $\mathcal{H}$ is not only identical with the monoclinic space group $\mathcal{G}$ considered but it also has the same Hermann–Mauguin symbol. The vectors $\mathbf{a} = \mathbf{a}'$ and $\mathbf{b} = \mathbf{b}'$ of the monoclinic basis are taken as basis vectors of the lattices of sectional layer groups and the vector $\mathbf{c} = \mathbf{d}$ defines the scanning direction.

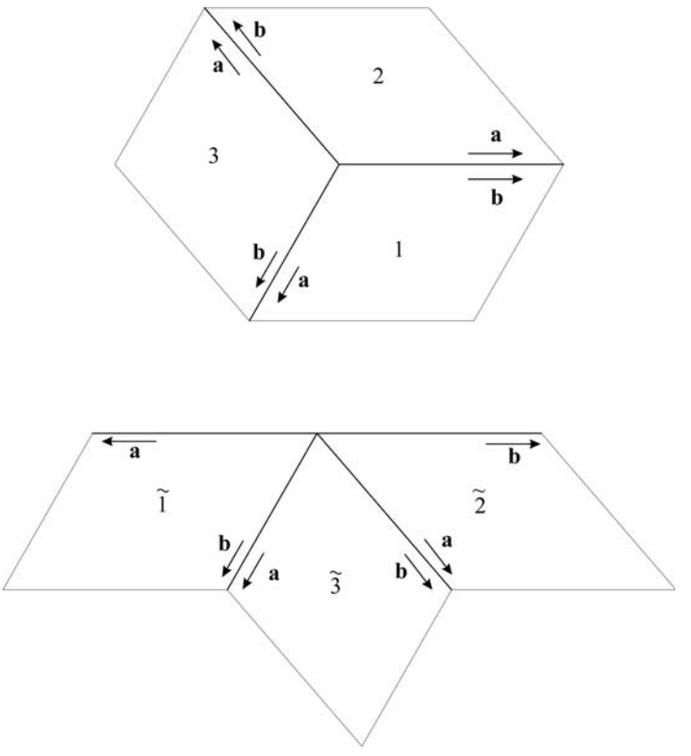

Fig. 5.2.4.1. Six monoclinic cell choices.

The Hermann–Mauguin symbol of the scanned group $\mathcal{G}$ changes with reference to a basis in which the b axis is chosen as the unique axis. However, the Hermann–Mauguin symbol of the group in its role as the scanning group does not change, because the basis of the scanning group is chosen as $\mathbf{a}' = \mathbf{c}$, $\mathbf{b}' = \mathbf{a}$ and $\mathbf{d} = \mathbf{b}$.

Monoclinic/inclined scanning. There exists an infinite number of orientations for which the section planes are parallel with the unique axis. When the c axis is chosen as the unique axis, the orientations are specified by Miller indices $(mn0)$. Each orientation orbit contains again just one orientation and the scanning group $\mathcal{H}$ is identical with the space group $\mathcal{G}$. The lattice of each sectional layer group is either a primitive or centred rectangular lattice with basis vectors $\mathbf{a}' = \mathbf{c}$ and $\mathbf{b}' = n\mathbf{a} - m\mathbf{b}$. The scanning direction is generally inclined to this orientation and the vector $\mathbf{d}$ can be chosen as any vector of the form $\mathbf{d} = p\mathbf{a} + q\mathbf{b}$, where p, q are integers that satisfy the condition $nq + mp = 1$ so that the vectors $\mathbf{a}'$, $\mathbf{b}'$ and $\mathbf{d}$ constitute a conventional unit cell of the scanning group, see Section 5.2.2.3.

The Hermann–Mauguin symbols for the group $\mathcal{H} = \mathcal{G}$ in its role as the scanning group are different to the symbol that specifies it as the scanned group because they refer to the choice of basis where the unique axis is defined by the vector $\mathbf{a}'$. The choice of the pair of vectors $\mathbf{b}' = n\mathbf{a} - m\mathbf{b}$ and $\mathbf{d} = p\mathbf{a} + q\mathbf{b}$ defines a cell choice to which the Hermann–Mauguin symbol of the group $\mathcal{H} = \mathcal{G}$ as the scanning group refers. Notice that the vector $\mathbf{b}'$ is defined by Miller indices $(mn0)$ while freedom in the choice of the scanning direction $\mathbf{d}$ remains. The choice of vector $\mathbf{d}$ may influence the Hermann–Mauguin symbols of the scanning group and of the sectional layer groups but it does not change the groups.

When the b axis is chosen as the unique axis, the orientations of section planes are defined by Miller indices $(n0m)$ and the conventional basis of the scanning group is chosen as $\mathbf{a}' = \mathbf{b}$, $\mathbf{b}' = n\mathbf{c} - m\mathbf{a}$, $\mathbf{d} = pc + q\mathbf{a}$. The symbols of the group in its role as the scanning group for various parities of integers n, m, p and

q, the linear orbits and the sectional layer groups are the same as in the case of unique axis c.

The cases of monoclinic/inclined scanning appear in all groups of higher symmetries than monoclinic for those orientations for which the scanning group is monoclinic. These cases are collected in the auxiliary tables where reference to the monoclinic/inclined part of the monoclinic scanning tables is given in each particular case.

5.2.4.3. *Orthorhombic system*

All groups of the orthorhombic system belong to Laue class *mmm* (D_{2h}). The standard-format tables are given first for the geometric classes 222 (D_2), *mm*2 (C_{2v}) and *mmm* (D_{2h}). These are followed by the auxiliary tables.

5.2.4.3.1. *Orthogonal scanning, standard tables*

Orientation orbits (001), (100) and (010): These three orientation orbits represent all orbits with fixed parameters in the orthorhombic system. Each of these consists of a single orientation. Hence the scanning group $\mathcal{H}$ for each of these orientations and for any orthorhombic group $\mathcal{G}$ coincides with the group $\mathcal{G} = \mathcal{H}$ itself. The Hermann–Mauguin symbols of the scanning groups are, however, generally different for the three orientations because they refer to different bases $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}' = \mathbf{d}$. For the orientation (001) they always coincide with the Hermann–Mauguin symbol used in *IT* A.

The scanning groups for groups of geometric classes 222 (D_2) and *mmm* (D_{2h}) are not only the same (identical with the scanned group) for all three orientations, but in a few cases they also have the same Hermann–Mauguin symbols, so the entries in the columns of the scanning group and of the sectional layer groups coincide. The orbits are separated by horizontal lines in the first column and further through the column with the scanning group, orbits and sectional layer groups, if they are different; when the Hermann–Mauguin symbol of the scanning group and hence the two remaining columns are identical, we give them as a common row for all the three orbits, which are then separated only in the first two columns. In the tables for groups of geometric class *mm*2 (C_{2v}), the orbit (001) is separated by double lines across the table from the remaining orbits (100) and (010), which are separated by single lines across the tables.

The bases for the scanning groups and for the sectional layer groups associated with these orbits are chosen in a standard manner for all orthorhombic groups:

(1) For the orientation (001), it is natural to choose $\mathbf{a}' = \mathbf{a}$, $\mathbf{b}' = \mathbf{b}$ and $\mathbf{c}' = \mathbf{d} = \mathbf{c}$. The symbol of the scanning group then coincides with the symbol of the space group itself, *i.e.* its symbol in the (*abc*) setting.

(2) The scanning direction for orientations (100) and (010) are along $\mathbf{d} = \mathbf{a}$ and $\mathbf{d} = \mathbf{b}$, respectively. We choose the remaining vectors $\mathbf{a}'$, $\mathbf{b}'$ in such a way that ($\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{d}$) is a right-handed basis, hence $\mathbf{a}' = \mathbf{b}$, $\mathbf{b}' = \mathbf{c}$ for the orientation (100) and $\mathbf{a}' = \mathbf{c}$, $\mathbf{b}' = \mathbf{a}$ for the orientation (010). Accordingly, the Hermann–Mauguin symbols for the scanning groups are the symbols which correspond to the settings (*bac*) and ($\bar{c}\bar{a}b$), respectively.

5.2.4.3.2. *Inclined scanning, auxiliary tables*

Orientation orbits (*mn*0), (0*mn*) *and* (*n*0*m*): Each of these orientations has a scanning group of monoclinic symmetry, namely: 2 (C_2) for space groups of the geometric class 222 (D_2) in all settings and for the groups of the class *mm*2 (C_{2v}) in the (*abc*) setting; *m* (C_s) for groups of the geometric class *mm*2 (C_{2v}) in the settings (*bac*), ($c\bar{a}b$); and 2/*m* (C_{2h}) for groups of the geometric class *mmm* (D_{2h}) in all settings. In each case, the scanning group $\mathcal{H}$ is a halving subgroup of the scanned group $\mathcal{G}$ and consequently each orientation orbit contains two orientations with the same scanning group. The symmetry increases to orthorhombic and the orbit contains one orientation for the special values $m = \pm 1$, $n = 0$ or $m = 0$, $n = \pm 1$.

The scanning groups are monoclinic and one can deduce them by viewing the diagrams of the scanned groups. By omitting the axes parallel with and planes perpendicular to the diagram plane, the diagram of the scanning group remains. This, however, is the diagram of the monoclinic scanning group in its standard setting when the unique axis is perpendicular to the plane of the diagram. This unique axis is a common direction for both orientations of the orbit and it is the c axis for the orientation orbit (*mn*0), and the a axis and b axis for the orientation orbits (0*mn*) and (*n*0*m*), respectively. The basis $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{d}$ for the scanning group is expressed in the same way through the auxiliary basis and the scanning groups in the reference tables are given by their Hermann–Mauguin symbols with reference to the auxiliary bases. The three orbits are separated by horizontal lines in the tables of orientation orbits as well as in the first column of the reference tables. If the scanning group in a column for a certain scanned group $\mathcal{G}$ has the same symbol for orbits in adjoining rows, we give it in a block common to these orbits.

Transformation of Miller indices for centred cases: In the table of orientation orbits for the C centring, we denote the orientation of the first orbit by (hk0) and ($\bar{h}k$0), *i.e.* we use letters h and k instead of m and n. The letters m and n are used for the Miller indices with respect to an auxiliary basis.

The scanning group is an equitranslational subgroup of the orthorhombic scanned group. Since the scanning group is monoclinic, the orthorhombic C lattice is considered as a monoclinic P lattice (with degenerate parameters) for which we choose the auxiliary basis vectors as $\widehat{\mathbf{a}} = (\mathbf{a} - \mathbf{b})/2$, $\widehat{\mathbf{b}} = (\mathbf{a} + \mathbf{b})/2$ and the unique axis vector $\widehat{\mathbf{c}} = \mathbf{c}$.

The orientations are, however, defined by Miller indices (hk0) with respect to the conventional basis ($\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$) of the orthorhombic group, while the numbers m, n define the Miller indices (*mn*0) with respect to the auxiliary basis ($\widehat{\mathbf{a}}$, $\widehat{\mathbf{b}}$, $\widehat{\mathbf{c}}$). The scanning can be found at once from tables of scanning of monoclinic groups in terms of parities of m, n, and of p, q, where $\mathbf{b}' = n\widehat{\mathbf{a}} - m\widehat{\mathbf{b}}$ is determined by the orientation (hk0) and p, q determine the scanning direction $\mathbf{d} = p\widehat{\mathbf{a}} + q\widehat{\mathbf{b}}$. Substituting for $\widehat{\mathbf{a}}$, $\widehat{\mathbf{b}}$ in vectors $\mathbf{b}'$ and $\mathbf{d}$, we get

$$\widehat{\mathbf{b}} = \frac{n-m}{2}\mathbf{a} - \frac{n+m}{2}\mathbf{b} = k\mathbf{a} - h\mathbf{b}, \tag{5.2.4.1}$$

so

$$k = \frac{n-m}{2}, \quad h = \frac{n+m}{2} \tag{5.2.4.2}$$

and conversely

$$n = h + k, \quad m = k - h. \tag{5.2.4.3}$$

If h is even and k odd, or h odd and k even, then both n and m are odd. However, if both h and k are odd (they cannot be simultaneously even), then both n and m are even, so that they cannot play the role of Miller indices, though they give the correct direction of the vector $\mathbf{b}'$. Dividing both by two, we get the Miller indices ($\frac{n}{2}\frac{m}{2}0$) and either the case $\frac{n}{2}$ odd, $\frac{m}{2}$ even or the case $\frac{n}{2}$ even, $\frac{m}{2}$ odd may occur. Both $\frac{n}{2}$ and $\frac{m}{2}$ cannot be simultaneously either even or odd because in these cases both h and k will be even.

The same situation occurs for the orbit (0*mn*) of A-centred orthorhombic groups of the class *mm*2 (C_{2v}), where the vector $\mathbf{a}$ plays the role of the unique monoclinic axis and for all three orientation orbits (*mn*0), (0*mn*) and (*n*0*m*) in the case of F-centred orthorhombic groups. In the latter case, the monoclinic scanning group is of the I-centred type with respect to the auxiliary bases while its centring in the bases ($\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{d}$) depends on the choice of n, m (*via* h, k), and of p, q, see the monoclinic cases.

Whenever a transformation of Miller indices is used, it is printed in a special row across the table below the respective orbit; the transformation is the same for all three orbits in the case of F centring and is given once below the orbits.

5.2.4.4. *Tetragonal system*

The scanning in the tetragonal system has a slightly different character for groups of Laue class $4/m$ (C_{4h}) from those of Laue class $4/mmm$ (D_{4h}).

5.2.4.4.1. *Orthogonal scanning, standard tables*

Orientation orbit (001): This orbit with a single special orientation appears in all tetragonal groups. In each case, the tetragonal group itself is the scanning group for this orientation. For those tetragonal groups that are presented in *IT* A with two origin choices, we specify the scanning group by its Hermann–Mauguin symbol and origin choice in parentheses (usually below the symbol). The scanning groups are expressed with respect to bases identical with the original basis, so that the Hermann–Mauguin symbol of the scanning group is identical with the Hermann–Mauguin symbol of the scanned group including the origin choice, $\mathbf{a}' = \mathbf{a}$, $\mathbf{b}' = \mathbf{b}$ are the vectors of the conventional basis for the sectional layer groups and the scanning direction $\mathbf{d} = \mathbf{c}$ is along the main axis. In the same way, we will later refer to tetragonal scanning groups when performing the scanning of cubic groups. There are no other orientation orbits with fixed parameters for groups of classes 4 (C_4), $\bar{4}$ (S_4) and $4/m$ (C_{4h}), *i.e.* for the groups of Laue class $4/m$ (C_{4h}).

Orientation orbit (100): This orbit contains orientations (100) and (010); it appears in groups of geometric classes 422 (D_4), $4mm$ (C_{4v}), $\bar{4}2m$ or $\bar{4}m2$ (D_{2d}), and $4/mmm$ (D_{4h}), which belong to the Laue class $4/mmm$ (D_{4h}), but not in the groups of Laue class $4/m$ (C_{4h}). We choose the bases of scanning groups as $\mathbf{a}' = \mathbf{b}$, $\mathbf{b}' = \mathbf{c}$, $\mathbf{d} = \mathbf{a}$ for the orientation (100) and as $\mathbf{a}' = -\mathbf{a}$, $\mathbf{b}' = \mathbf{c}$, $\mathbf{d} = \mathbf{b}$ for the orientation (010). The corresponding scanning groups are orthorhombic and of the same centring type as the scanned group. In the majority of cases, the scanning groups are the same (*i.e.* expressed by the same Hermann–Mauguin symbol, with or without a shift) with respect to the two coordinate systems (P; $\mathbf{a}' = \mathbf{b}$, $\mathbf{b}' = \mathbf{c}$, $\mathbf{d} = \mathbf{a}$) and (P; $\mathbf{a}' = -\mathbf{a}$, $\mathbf{b}' = \mathbf{c}$, $\mathbf{d} = \mathbf{b}$) where P is the origin of the original group. In these cases, only one Hermann–Mauguin symbol (with or without a shift) is given for both orientations and one corresponding column of linear orbits and of sectional layer groups. Whenever this is not the case, the scanning group for one of the orientations is shifted with reference to its coordinate system as compared with the location of the other scanning group with reference to its coordinate system. There is also a respective shift of orientation orbits and of corresponding sectional layer groups. In these cases, the orientation-orbit row is split into two parts, each referring to one orientation of the orbit.

Orientation orbit (110): The orbit contains the orientations (110) and (1$\bar{1}$0); it again appears in all groups of the geometric classes 422 (D_4), $4mm$ (C_{4v}), $\bar{4}2m$ (D_{2d}) and $4/mmm$ (D_{4h}) belonging to the Laue class $4/mmm$ (D_{4h}), but not in the groups of Laue class $4/m$ (C_{4h}). We choose the bases of scanning groups as $\mathbf{a}' = (-\mathbf{a} + \mathbf{b})$, $\mathbf{b}' = \mathbf{c}$, $\mathbf{d} = (\mathbf{a} + \mathbf{b})$ for the orientation (1$\bar{1}$0) and as $\mathbf{a}' = (\mathbf{a} + \mathbf{b})$, $\mathbf{b}' = \mathbf{c}$, $\mathbf{d} = (\mathbf{a} - \mathbf{b})$ for the orientation (1$\bar{1}$0). The resulting scanning groups are again orthorhombic of centring type C (denoted by B in view of the choice of the basis) when the original tetragonal group is of the type P and of centring type F when the original tetragonal group is of the type I. The scanning group, respective linear orbits and sectional layer groups are either the same with reference to the coordinate systems (P; $\mathbf{a}' = (-\mathbf{a} + \mathbf{b})$, $\mathbf{b}' = \mathbf{c}$, $\mathbf{d} = (\mathbf{a} + \mathbf{b})$) and ($P$; $\mathbf{a}' = (\mathbf{a} + \mathbf{b})$, $\mathbf{b}' = \mathbf{c}$, $\mathbf{d} = (\mathbf{a} - \mathbf{b})$) or one of them is shifted with respect to the other. Accordingly, the row for the orbit either does not split or it splits into two subrows for the two orientations.

5.2.4.4.2. *Inclined scanning, auxiliary tables*

Orientation orbits ($mn0$) occur in groups of both tetragonal Laue classes $4/m$ (C_{4h}) and $4/mmm$ (D_{4h}). Orientation orbits ($0mn$) occur only in groups of the Laue class $4/mmm$ (D_{4h}).

Orientation orbits ($mn0$): These orbits contain two orientations, namely $\pm(mn0)$ and $(\bar{n}m0)$ in groups of the geometric classes 4 (C_4), $\bar{4}$ (S_4) and $4/m$ (C_{4h}) which belong to the Laue class $4/m$ (C_{4h}), and four orientations, namely ($mn0$), ($\bar{n}m0$), ($\bar{m}n0$) and ($nm0$) in groups of the geometric classes 422 (D_4), $4mm$ (C_{4v}), $\bar{4}2m$ (D_{2d}) and $4/mmm$ (D_{4h}) which belong to the Laue class $4/mmm$ (D_{4h}).

For special values $m = 1$ and $n = 0$, the orbit contains only two orientations (100) and (010) which form an orbit with fixed parameters with an orthorhombic scanning group for groups of the Laue class $4/mmm$ (D_{4h}). For groups of the Laue class $4/m$ (C_{4h}) these two orientations represent just one particular case of the orbit ($mn0$). Analogously, the orbit with two orientations (110) and (1$\bar{1}$0) for groups of the Laue class $4/mmm$ (D_{4h}) is an orbit with fixed parameters $m = 1$, $n = 1$ while for groups of the Laue class $4/m$ (C_{4h}) it is a particular case of the orbits ($mn0$).

There are no other special orbits with variable parameter in groups of the Laue class $4/m$ (C_{4h}). Auxiliary bases are defined by one table common for both centring types P and I.

Auxiliary bases for this orbit are also common for both centring types in groups of the Laue class $4/mmm$ (D_{4h}) and they are given in the tables of orientation orbits for both types.

Orientation orbits ($0mn$): These orbits, consisting of orientations ($0mn$), ($0\bar{m}n$), ($m0n$) and ($m0\bar{n}$), appear only in groups of the Laue class $4/mmm$ (D_{4h}). The first two orientations contain the vector $\mathbf{a}$, the other two contain the vector $\mathbf{b}$, scanning groups are monoclinic with unique axes along vectors $\mathbf{a}$ and $\mathbf{b}$, respectively, for the first and second pair of orientations; the scanning is inclined because the vectors $\mathbf{a}$ and $\mathbf{b}$ lie in the respective orientations. To primitive and centred lattices of the scanned groups there correspond primitive and centred lattices of the scanning groups, respectively, which is reflected in the reference tables.

Auxiliary bases for this orbit are common for both centring types in groups of the Laue class $4/mmm$ (D_{4h}) and they are given in tables of orientation orbits for both types.

For special values of parameters, the orbit coincides either with the orbit (100), (010) or with the orbit (110), (1$\bar{1}$0).

Orientation orbits (hhl): These orbits, consisting of orientations (hhl), ($\bar{h}\bar{h}l$), ($h\bar{h}l$) and ($\bar{h}hl$), appear again only in groups of the Laue class $4/mmm$ (D_{4h}). The first two orientations contain the vector $(\mathbf{a} - \mathbf{b})$, the other two contain the vector $(\mathbf{a} + \mathbf{b})$, scanning groups are monoclinic with unique axes along these vectors $(\mathbf{a} - \mathbf{b})$ and $(\mathbf{a} + \mathbf{b})$, respectively, for the first and second pair of orientations; the scanning is again inclined because the vectors $(\mathbf{a} - \mathbf{b})$ and $(\mathbf{a} + \mathbf{b})$ lie in the respective orientations.

The auxiliary bases for the monoclinic scanning groups in the case of a primitive (P) tetragonal lattice are chosen as

$$\widehat{\mathbf{a}} = \mathbf{a} + \mathbf{b}, \quad \widehat{\mathbf{b}} = \mathbf{c} \quad \text{and} \quad \widehat{\mathbf{c}} = \mathbf{a} - \mathbf{b} \tag{5.2.4.4}$$

for the first pair of orientations and as

$$\widehat{\mathbf{a}} = \mathbf{b} - \mathbf{a}, \quad \widehat{\mathbf{b}} = \mathbf{c} \quad \text{and} \quad \widehat{\mathbf{c}} = \mathbf{a} + \mathbf{b} \tag{5.2.4.5}$$

for the second pair of orientations.

The auxiliary bases for the monoclinic scanning groups in the case of an I-centred tetragonal lattice are chosen as

$$\widehat{\mathbf{a}} = (\mathbf{a} + \mathbf{b} + \mathbf{c})/2, \quad \widehat{\mathbf{b}} = \mathbf{c} \quad \text{and} \quad \widehat{\mathbf{c}} = (\mathbf{a} - \mathbf{b}) \tag{5.2.4.6}$$

for the first pair of orientations and as

$$\widehat{\mathbf{a}} = (\mathbf{b} - \mathbf{a} + \mathbf{c})/2, \quad \widehat{\mathbf{b}} = \mathbf{c} \quad \text{and} \quad \widehat{\mathbf{c}} = (\mathbf{a} + \mathbf{b}) \tag{5.2.4.7}$$

for the second pair of orientations.

A vector parallel with planes of orientation (hhl) and orthogonal to $\mathbf{a} - \mathbf{b}$ is a multiple of

$$2h\mathbf{c} - l(\mathbf{a} + \mathbf{b}). \quad (5.2.4.8)$$

In terms of Miller indices ($mn0$) with reference to the first auxiliary basis for a P-centred lattice, such a vector is a multiple of

$$m\mathbf{c} - n(\mathbf{a} + \mathbf{b}) \quad (5.2.4.9)$$

and in terms of Miller indices ($mn0$) with reference to the first auxiliary basis for an I-centred lattice, it is a multiple of

$$(2m - n)\mathbf{c} - n(\mathbf{a} + \mathbf{b}). \quad (5.2.4.10)$$

Therefore, for a P-centred lattice, the pair of numbers (m, n) must be proportional to the pair $(2h, l)$. Since Miller indices must be relatively prime, we get $n = l$, $m = 2h$ if l is odd and $n = l/2$, $m = h$ if l is even.

For an I-centred lattice, the pair of numbers $(2m - n, n)$ must be proportional to the pair $(2h, l)$ and hence the pair $(2m, n)$ must be proportional to the pair $(2h + l, l)$. If l is odd, then $2h + l$ is also odd and we put $m = 2h + l$, so that $n = 2l$. If l is even, we put $n = l$ and $m = h + l/2$.

These relations are printed in the last rows across the tables of orientation orbits within the block for orbit (hhl).

5.2.4.5. *Hexagonal family*

The family splits into the trigonal and the hexagonal system. With the exception of seven group types with rhombohedral lattices [$R3$, C_3^4 (No. 146); $R\bar{3}$, C_{3i}^2 (No. 148); $R32$, D_3^7 (No. 155); $R3m$, C_{3v}^5 (No. 160); $R3c$, C_{3v}^6 (No. 161); $R\bar{3}m$, D_{3d}^5 (No. 166); and $R\bar{3}c$, D_{3d}^6 (No. 167)] all space groups of both systems have a primitive hexagonal lattice. Scanning tables are given in the hexagonal coordinate system for all groups with this lattice and the bases of the scanning groups for individual orientations are chosen identically. For the seven groups with rhombohedral lattices, the description of scanning in the hexagonal coordinate system differs from the description in the rhombohedral coordinate system only in the specification of orientations by Bravais–Miller and Miller indices, respectively. The column *Orientation orbit* is split into two columns with the headings HEXAG. AXES and RHOMB. AXES.

5.2.4.5.1. *Orthogonal scanning, standard tables*

Orientation orbit (0001): The orientation (0001) is invariant under all point groups of the family; it forms therefore an orientation orbit with a single special orientation in all space groups of the family and the scanning groups for this orientation coincide with the scanned groups. We choose $\mathbf{a}' = \mathbf{a}$, $\mathbf{b}' = \mathbf{b}$, $\mathbf{d} = \mathbf{c}$ in primitive as well as in rhombohedral cases; in the latter case, the orientation is also specified in the second column as (111). The Hermann–Mauguin symbols of the scanning groups also coincide with the symbols of the scanned groups; to specify both the scanned and the scanning groups with rhombohedral lattices with reference to hexagonal bases we use an obverse setting as in *IT* A.

All corresponding sectional layer groups have the same planar hexagonal lattice with basis vectors $\mathbf{a}' = \mathbf{a}$ and $\mathbf{b}' = \mathbf{b}$. The basis $(\mathbf{a}, \mathbf{b})$, denoted as usual by p, is the conventional basis for all trigonal/hexagonal, hexagonal/hexagonal, monoclinic/oblique and triclinic/oblique sectional layer groups. To describe the monoclinic/rectangular and orthorhombic/rectangular sectional layer groups, we choose three conventional rectangular bases: $\widehat{c}_1 = (\mathbf{a}, \mathbf{a} + 2\mathbf{b})$, $\widehat{c}_2 = (\mathbf{b}, -(2\mathbf{a} + \mathbf{b}))$ and $\widehat{c}_3 = (-(\mathbf{a} + \mathbf{b}), (\mathbf{a} - \mathbf{b}))$, as shown in Fig. 5.2.4.2. The symbols $\widehat{c}_1, \widehat{c}_2, \widehat{c}_3$ then denote the same lattice, identical with the p-lattice with the conventional basis $(\mathbf{a}, \mathbf{b})$.

In the cases of the trigonal space-group types $P3_112$, D_3^3 (No. 151), $P3_121$, D_3^4 (No. 152), $P3_212$, D_3^5 (No. 153) and $P3_221$, D_3^6 (No. 154), and in the cases of the hexagonal space-group types $P6_122$, D_6^2 (No. 178) and $P6_522$, D_6^3 (No. 179), there exist two linear orbits with fixed parameter for which the sectional layer groups are monoclinic/rectangular with a c-centred lattice. The orientations of the unique axes of the respective monoclinic/rectangular groups are then defined by the choice of the conventional basis to which the Hermann–Mauguin symbol refers (*i.e.* by index in $\widehat{c}_1$, $\widehat{c}_2$ or $\widehat{c}_3$) and by the position of the twofold rotation in the symbol. In group types $P6_222$, D_6^4 (No. 180) and $P6_422$, D_6^5 (No. 181) there exist two linear orbits with fixed parameters for which the sectional layer groups are orthorhombic/rectangular with a c-centred lattice. The orientations of twofold axes of orthorhombic/rectangular groups in the section plane are again defined by the conventional bases $\widehat{c}_1, \widehat{c}_2$ or $\widehat{c}_3$. There are no other non-trivial orientation orbits in groups of the Laue class $\bar{3}$ (C_{3i}) and no other orbits with fixed parameters in groups of the Laue class $6/m$ (C_{6h}).

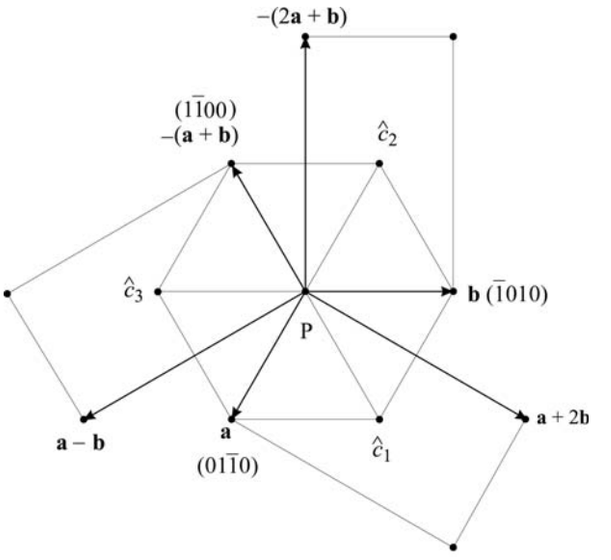

Fig. 5.2.4.2. Symbols for a hexagonal lattice with a rectangular point group.

Orientation orbits (01$\bar{1}$0) *and* ($\bar{1}$2$\bar{1}$0): These two orbits appear in all biaxial groups of the trigonal and hexagonal system, *i.e.* in groups of the Laue classes $\bar{3}m$ (D_{3d}) and $6/mmm$ (D_{6h}). We consider them together because corresponding scanning groups for pairs of orientations, one from each of these orbits, are related in the same way to their corresponding bases.

Hexagonal lattice. If the scanned group is trigonal with a primitive hexagonal lattice, the scanning group is monoclinic; if

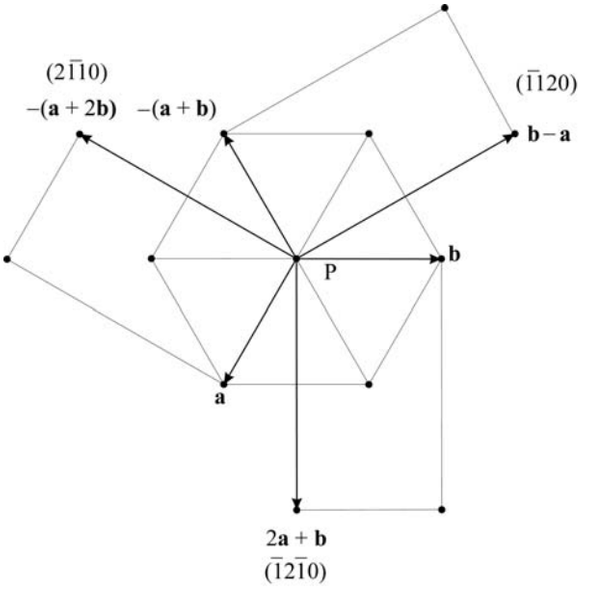

Fig. 5.2.4.3. Another choice of orthogonal basis vectors for a hexagonal lattice.

the scanned group is hexagonal, the scanning group is orthorhombic with lattice type *C*. Because of the choice of bases, the lattice is denoted by the letter *A* in the Hermann–Mauguin symbols of the scanning groups.

We choose the vector **c** of the hexagonal axis as the vector $\mathbf{a}'$ for all orientations of these orbits. In addition we choose $\mathbf{b}' = \mathbf{a}$ and the scanning direction $\mathbf{d} = \mathbf{a} + 2\mathbf{b}$ for the orientation $(01\bar{1}0)$, while for the orientation $(2\bar{1}\bar{1}0)$, perpendicular to it, we choose $\mathbf{b}' = -(\mathbf{a} + 2\mathbf{b})$, $\mathbf{d} = \mathbf{a}$. Analogously, for the other pairs of mutually perpendicular orientations we choose: $\mathbf{b}' = \mathbf{b}$ and $\mathbf{d} = -(2\mathbf{a} + \mathbf{b})$ for the orientation $(\bar{1}010)$; $\mathbf{b}' = 2\mathbf{a} + \mathbf{b}$, $\mathbf{d} = \mathbf{b}$ for the orientation $(\bar{1}2\bar{1}0)$; $\mathbf{b}' = -(\mathbf{a} + \mathbf{b})$, $\mathbf{d} = (\mathbf{a} - \mathbf{b})$ for the orientation $(1\bar{1}00)$; and $\mathbf{b}' = (\mathbf{b} - \mathbf{a})$, $\mathbf{d} = -(\mathbf{a} + \mathbf{b})$ for the orientation $(\bar{1}\bar{1}20)$. Hence the scanning groups for the pairs of orientations $(01\bar{1}0)/(2\bar{1}\bar{1}0)$, $(\bar{1}010)/(\bar{1}2\bar{1}0)$ and $(1\bar{1}00)/(\bar{1}\bar{1}20)$ are the same monoclinic or orthorhombic groups but the conventional basis vectors $\mathbf{b}'$, $\mathbf{d}$ of one of them are replaced by $-\mathbf{d}$, $\mathbf{b}'$, respectively, for the second one. Again there are cases when the locations of scanning groups are different for different pairs of orientations, in which case the corresponding row splits into three subrows. To compare the geometry of the bases, consult and compare Figs. 5.2.4.2 and 5.2.4.3.

Rhombohedral lattice. The resulting scanning groups are monoclinic of the *I*-centred type. The vectors of the rhombohedral basis $\mathbf{a}_r$, $\mathbf{b}_r$, $\mathbf{c}_r$ are related to vectors **a**, **b**, **c** of the hexagonal basis as follows:

$$\mathbf{a}_r = (2\mathbf{a} + \mathbf{b} + \mathbf{c})/3, \quad \mathbf{b}_r = (-\mathbf{a} + \mathbf{b} + \mathbf{c})/3,$$
$$\mathbf{c}_r = (-\mathbf{a} - 2\mathbf{b} + \mathbf{c})/3, \qquad (5.2.4.11)$$

as shown in Fig. 5.2.4.4, which corresponds to the obverse setting. In Figs. 5.2.4.5 and 5.2.4.6, we show the diagrams of the scanning groups in the plane of orientation $(\bar{1}2\bar{1}0)$ for the groups $R\bar{3}m$, D_{3d}^5 (No. 166) and $R\bar{3}c$, D_{3d}^6 (No. 167), projected orthogonally along the direction of **b**. The vector $(\mathbf{a}_r + \mathbf{b}_r)$, whose projection is shown in both figures, is identical with the vector $(\mathbf{a}_r + \mathbf{b} + \mathbf{c})/2$ which is the *I*-centring vector of the monoclinic cell with conventional basis $\mathbf{a}' = \mathbf{c}$, $\mathbf{b}' = \mathbf{a}_r$, $\mathbf{d} = \mathbf{b}$. The vector **b** plays the role of the scanning direction for orientation $(\bar{1}2\bar{1}0)$ to which it is perpendicular (this is the case of monoclinic/orthogonal scanning). For the orientation $(\bar{1}010)$, we choose the basis of the scanning group as $\mathbf{a} = \mathbf{c}$, $\mathbf{b}' = \mathbf{b}$ and $\mathbf{d} = -\mathbf{a}_r$, and we get a monoclinic/inclined scanning.

One standard scanning table is given for each of the seven group types with a rhombohedral lattice because neither the bases of scanning groups nor their symbols change with the change from hexagonal to rhombohedral basis. None of the entries in the scanning tables needs to be changed with the exception of Bravais–Miller indices (*hkil*), which are replaced by corresponding Miller indices (*hkl*) as follows: (0001) is replaced by (111), the set $(01\bar{1}0)$, $(\bar{1}010)$, $(1\bar{1}00)$ by $(11\bar{1})$, $(\bar{1}11)$, $(1\bar{1}1)$ and the set $(\bar{1}2\bar{1}0)$, $(\bar{1}\bar{1}20)$, $(2\bar{1}\bar{1}0)$ by $(01\bar{1})$, $(\bar{1}01)$, $(1\bar{1}0)$. The indices are given in parallel in the two columns for the designation of orientation orbits. To abbreviate expressions for vectors of the conventional bases $(\mathbf{a}', \mathbf{b}', \mathbf{d})$ of scanning groups, we express these vectors in terms of vectors of hexagonal basis $(\mathbf{a}, \mathbf{b}, \mathbf{c})$ and of vectors of rhombohedral basis $(\mathbf{a}_r, \mathbf{b}_r, \mathbf{c}_r)$. To obtain the bases $(\mathbf{a}', \mathbf{b}', \mathbf{d})$ in terms of vectors of the hexagonal basis, we substitute for vectors of the rhombohedral bases the combinations (5.2.4.11), to obtain them in terms of vectors of rhombohedral bases, we substitute for vectors of hexagonal bases the combinations

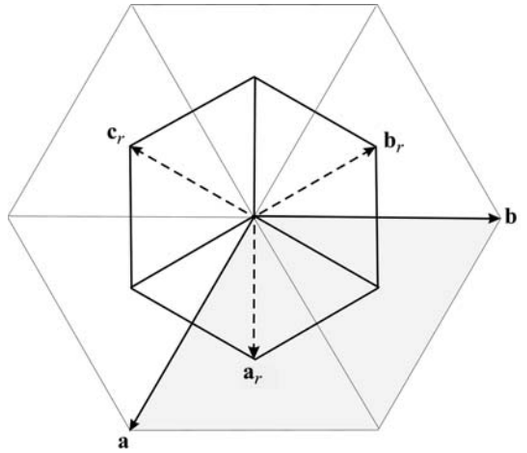

Fig. 5.2.4.4. The relationship between hexagonal and rhombohedral bases in the obverse setting.

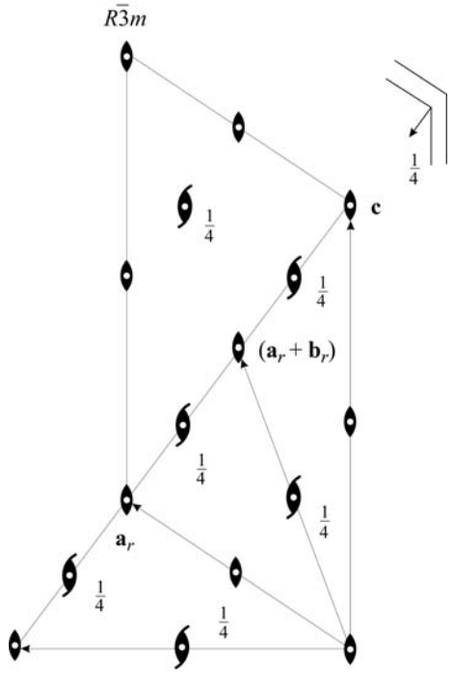

Fig. 5.2.4.5. The diagram of the scanning group $R\bar{3}m$ in the plane of orientation $(\bar{1}2\bar{1}0)$ projected orthogonally along **b**.

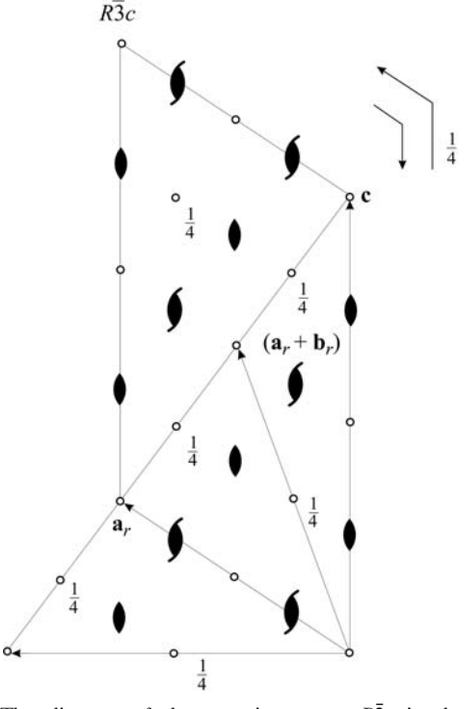

Fig. 5.2.4.6. The diagram of the scanning group $R\bar{3}c$ in the plane of orientation $(\bar{1}2\bar{1}0)$ projected orthogonally along **b**.

$$\mathbf{a} = \mathbf{a}_r - \mathbf{b}_r, \quad \mathbf{b} = \mathbf{b}_r - \mathbf{c}_r, \quad \mathbf{c} = \mathbf{a}_r + \mathbf{b}_r + \mathbf{c}_r, \qquad (5.2.4.12)$$

reciprocal to (5.2.4.11).

5.2.4.5.2. *Inclined scanning, auxiliary tables*

There are no orientation orbits with variable parameter and hence no auxiliary tables to the Laue class $\bar{3}$ (C_{3i}).

Orientation orbit ($mn\,\overline{m+n}\,0$): This orbit appears in groups of the Laue class $6/m$ (C_{6h}), where it contains the three orientations ($mn\,\overline{m+n}\,0$), ($\overline{m+n}\,mn0$) and ($n\,\overline{m+n}\,m0$); further, it appears in groups of the Laue class $6/mmm$ (D_{6h}), where it contains six orientations – to the three orientations we add their images generated by auxiliary axes or planes, which are the orientations ($nm\,\overline{m+n}\,0$), ($\overline{m+n}\,nm0$) and ($m\,\overline{m+n}\,n0$). The choice of basis vectors for the scanning group of the first orientation ($mn\,\overline{m+n}\,0$) is: $\mathbf{a}' = \mathbf{c}$, $\mathbf{b}' = n\mathbf{a} - m\mathbf{b}$ and $\mathbf{d} = p\mathbf{a} + q\mathbf{b}$; as always in monoclinic/inclined scanning, the bases for other orientations are obtained by rotations around the principal axis [Laue class $6/m$ (C_{6h})] and by reflections in auxiliary planes [Laue class $6/mmm$ (D_{6h})], so that the scanning groups and the scanning are expressed by identical symbols in their respective bases.

For the particular values $m = 0$, $n = 1$ or $m = -1$, $n = 2$, the orientation orbit turns into a special orbit ($01\bar{1}0$) or ($\bar{1}2\bar{1}0$) with fixed parameters, respectively, for which the scanning group and hence the scanning is orthorhombic.

Orientation orbits ($0h\bar{h}l$) and ($\bar{h}2h\bar{h}l$): These two orbits include those orientations which contain the secondary or tertiary directions of the hexagonal system. Both orbits exist in the Laue classes $\bar{3}m$ (D_{3d}) and $6/mmm$ (D_{6h}); the orbit ($0h\bar{h}l$) appears in the arithmetic classes $321P$, $3m1P$, $\bar{3}m1P$ and $32R$, $3mR$, $\bar{3}mR$, where it contains further the two orientations ($\bar{h}0hl$) and ($h\bar{h}0l$); the orbit ($\bar{h}2h\bar{h}l$) appears in the arithmetic classes $312P$, $31mP$ and $\bar{3}1mP$, where it contains the two other orientations ($\overline{hh}2hl$), ($2h\overline{hh}l$): both orbits appear in all groups of the Laue class $6/mmm$ (D_{6h}) where they contain additional triplets of orientations: ($0h\overline{hl}$), ($\bar{h}0h\bar{l}$) and ($h\bar{h}0\bar{l}$) in the first case and ($\bar{h}2h\overline{hl}$), ($\overline{hh}2h\bar{l}$) and ($2h\overline{hh}l$) in the second case.

Transformation of Bravais–Miller indices: hexagonal axes. The orientations ($0h\bar{h}l$) are specified by Bravais–Miller indices with reference to the hexagonal basis ($\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$) through integers h, l. To find their Miller indices ($mn0$) with reference to auxiliary bases ($\widehat{\mathbf{a}}$, $\widehat{\mathbf{b}}$, $\widehat{\mathbf{c}}$), we consider a vector $\mathbf{w} = \mathbf{u} + \mathbf{v} \approx [l(\mathbf{a} + 2\mathbf{b}) - 2h\mathbf{c}]$ as shown in Fig. 5.2.4.7. This vector is proportional to a vector $\mathbf{b}'$, which is used as a vector of the conventional basis ($\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{d}$) of the scanning group in both centring types P and R. Vector $\mathbf{b}'$ is defined as $\mathbf{b}' = n\widehat{\mathbf{a}} - m\widehat{\mathbf{b}}$, where $\widehat{\mathbf{a}} = \mathbf{a} + 2\mathbf{b}$ for both the centring types P and R, while $\widehat{\mathbf{b}} = \mathbf{c}$ for the centring type P and $\widehat{\mathbf{b}} = \mathbf{c}_r$ for the centring type R.

The proportionality relations therefore read for the centring type P

$$l(\mathbf{a} + 2\mathbf{b}) - 2h\mathbf{c} \approx n(\mathbf{a} + 2\mathbf{b}) - m\mathbf{c}, \qquad (5.2.4.13)$$

from which we express n, m through h, l as follows:

$$l \text{ odd } \Rightarrow n = l, m = 2h; \quad l \text{ even } \Rightarrow n = l/2, m = h.$$

In the case of the centring type R, we have

$$\begin{aligned}\mathbf{b}' &= n(\mathbf{a} + 2\mathbf{b}) - m(-\mathbf{a} - 2\mathbf{b} + \mathbf{c})/3 \\ &= (n + m/3)(\mathbf{a} + 2\mathbf{b}) - m\mathbf{c}/3,\end{aligned}$$

so that the proportionality relation reads

$$l(\mathbf{a} + 2\mathbf{b}) - 2h\mathbf{c} \approx (n + m/3)(\mathbf{a} + 2\mathbf{b}) - (m/3)\mathbf{c}. \qquad (5.2.4.14)$$

Comparing the coefficients, we obtain that the pair (n, m) must be proportional to the pair ($l - 2h$, $6h$), from which we express n, m through h, l as follows:

$$l \text{ odd } \Rightarrow n = l - 2h, m = 6h; \quad l \text{ even } \Rightarrow n = l/2 - h, m = 3h.$$

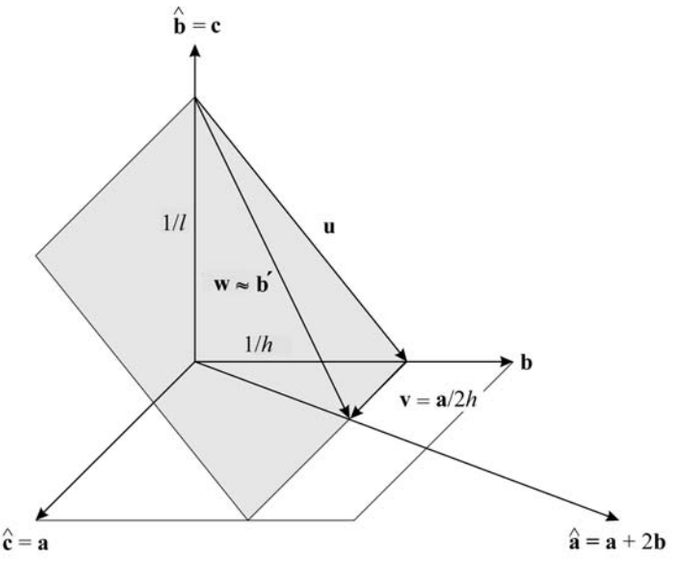

Fig. 5.2.4.7. Illustration of the transformation of Bravais–Miller indices in a hexagonal basis to Bravais indices in an auxiliary basis.

For the orientation orbit ($\bar{h}2h\bar{h}l$), we obtain the proportionality relation by comparing the proportional vectors $\mathbf{b}' = n\widehat{\mathbf{a}} - m\widehat{\mathbf{b}} = n\mathbf{b} - m\mathbf{c}$ and $l\mathbf{b} - 2h\mathbf{c}$, which leads again to the relations

$$l \text{ odd } \Rightarrow n = l, m = 2h; \quad l \text{ even } \Rightarrow n = l/2, m = h.$$

The relations between indices h, l and m, n are, as usual, recorded under each orbit in a row across the table.

The orientation orbits ($0h\bar{h}l$) and ($\bar{h}2h\bar{h}l$) turn into the special orbits ($01\bar{1}0$) and ($\bar{1}2\bar{1}0$) with fixed parameter for the special values $h = 1$, $l = 0$, and their symmetry increases to orthorhombic for groups of the Laue class $6/mmm$ (D_{6h}). In groups of the Laue class $\bar{3}m$ (D_{3d}), the symmetry of these orbits remains monoclinic but the scanning changes from monoclinic/inclined to monoclinic/orthogonal.

Rhombohedral axes. Auxiliary tables for the five group types with a rhombohedral lattice are given in a compact manner for all three arithmetic classes. Neither auxiliary nor conventional (in the sense of the convention for scanning groups, see Section 5.2.2.3) bases of scanning groups change. The orientations of the orbit are expressed by Bravais–Miller indices in the hexagonal basis and these are transformed to Miller indices ($mn0$) with reference to the auxiliary basis as shown above. In the rhombohedral basis, we describe orientations of the orbit by Miller indices (hhl). The integers h, l here are considered independently of the same letters in Bravais–Miller indices. To transform them into Miller indices with reference to the auxiliary basis, we take into account that the vector $\mathbf{w}$ from Fig. 5.2.4.7 is proportional to $l(\mathbf{a}_r + \mathbf{b}_r) - 2h\mathbf{c}_r$ as well as to $n(\mathbf{a}_r + \mathbf{b}_r + \mathbf{c}_r) - m\mathbf{c}_r = n(\mathbf{a}_r + \mathbf{b}_r) + (n - m)\mathbf{c}_r$. Comparing coefficients at ($\mathbf{a}_r + \mathbf{b}_r$) and $\mathbf{c}_r$ we obtain

$$l \text{ odd } \Rightarrow n = l, m = 2h + l; \quad l \text{ even } \Rightarrow n = l/2, m = h + l/2.$$

The reference table is given as a common table for consideration in hexagonal or rhombohedral axes. It is also common for all five group types with rhombohedral lattice for which this type of orientation orbit occurs.

5.2.4.6. *Cubic system*

The character of scanning is again different for groups of the geometric classes 23 (T) and $m\bar{3}$ (T_h) with no fourfold axes and for groups of the geometric classes 432 (O), $\bar{4}3m$ (T_d) and $m\bar{3}m$ (O_h) which contain fourfold axes.

The threefold axis along the direction [111] passes through the origin in all cubic groups, including the cases when two origin choices are used. Rotations around this axis therefore transform

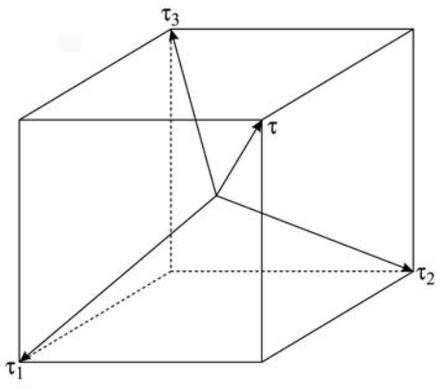

Fig. 5.2.4.8. Vectors along the main cubic axes.

the coordinate system in such a way that the conjugate scanning groups, linear orbits and sectional layer groups are expressed in the same way in the respective coordinate systems.

5.2.4.6.1. *Orthogonal scanning, standard tables*

Orientation orbit (001): This orientation orbit contains the orientations (001), (100) and (010). It appears in all cubic groups and it leads to orthorhombic scanning groups in the case of space groups of the classes 23 (T), $m\bar{3}$ (T_h) and to tetragonal scanning groups in the case of the classes 432 (O), $\bar{4}3m$ (T_d) and $m\bar{3}m$ (O_h). The conventional bases of the scanning groups for the orientation (001) are chosen as $\mathbf{a}' = \mathbf{a}$, $\mathbf{b}' = \mathbf{b}$, $\mathbf{d} = \mathbf{c}$ for all cases with the exception of F-centred types of groups of the classes 432 (O), $\bar{4}3m$ (T_d) and $m\bar{3}m$ (O_h). The centring types P, I and F remain the same for orthorhombic scanning groups, *i.e.* for the classes 23 (T) and $m\bar{3}$ (T_h), and for the P and I types of tetragonal scanning groups which apply to the classes 23 (O), $\bar{4}3m$ (T_d) and $m\bar{3}m$ (O_h). The F-centred type for the latter classes turns into I-centred tetragonal scanning groups with the conventional basis $\mathbf{a}' = (\mathbf{a} - \mathbf{b})/2$, $\mathbf{b}' = (\mathbf{a} + \mathbf{b})/2$, $\mathbf{d} = \mathbf{c}$ for the orientation (001).

For the remaining two orientations (100) and (010), we obtain the bases by the cyclic permutations $\mathbf{a} \to \mathbf{b} \to \mathbf{c} \to \mathbf{a}$ and $\mathbf{a} \to \mathbf{c} \to \mathbf{b} \to \mathbf{a}$, respectively, which correspond to rotations 3 and 3^2 around the threefold axis [111].

Orientation orbit (110): This orbit occurs only in groups of the classes 432 (O), $\bar{4}3m$ (T_d) and $m\bar{3}m$ (O_h). It consists of the orientations (110), $(1\bar{1}0)$, (011), $(01\bar{1})$, (101) and $(\bar{1}01)$. The scanning groups are orthorhombic in all cases. We choose the conventional basis of the scanning group as $\mathbf{a}' = \mathbf{c}$, $\mathbf{b}' = (\mathbf{a} - \mathbf{b})$, $\mathbf{d} = (\mathbf{a} + \mathbf{b})$ for the orientation $(11\bar{0})$ and as $\mathbf{a}' = \mathbf{c}$, $\mathbf{b}' = (\mathbf{a} + \mathbf{b})$, $\mathbf{d} = (\mathbf{b} - \mathbf{a})$ for the orientation $(1\bar{1}0)$ for the P- and I-centred cases. The corresponding scanning groups are orthorhombic of the centring types A and F, respectively. For the original F-centring, we choose the conventional basis of orthorhombic scanning groups as $\mathbf{a}' = \mathbf{c}$, $\mathbf{b}' = (\mathbf{a} - \mathbf{b})/2$, $\mathbf{d} = (\mathbf{a} + \mathbf{b})/2$ for the orientation (110) and as $\mathbf{a}' = \mathbf{c}$, $\mathbf{b}' = (\mathbf{a} + \mathbf{b})/2$, $\mathbf{d} = (\mathbf{a} - \mathbf{b})/2$ for the orientation $(1\bar{1}0)$, which results in I-centred orthorhombic scanning groups.

The bases for the scanning groups corresponding to the orientations (011) and $(01\bar{1})$ are obtained respectively by the cyclic permutation $\mathbf{a} \to \mathbf{b} \to \mathbf{c} \to \mathbf{a}$ and the bases of scanning groups for the orientations (101) and $(\bar{1}01)$ by the cyclic permutation $\mathbf{a} \to \mathbf{c} \to \mathbf{b} \to \mathbf{a}$, which again corresponds to the threefold rotations 3 and 3^2 around the [111] axis. Accordingly, the scanning groups, linear orbits and sectional layer groups are the same with reference to respective bases for the orientations (110), (011) and (101) as well as for the orientations $(1\bar{1}0)$, $(01\bar{1})$ and $(\bar{1}01)$. In some cases, there is also no difference between the two triplets of orientations and one row describes the scanning for all six orientations. In other cases, owing to fourfold screw axes, the scanning groups are shifted and the row splits into two subrows.

Orientation orbit (111): This orbit with orientations (111), $(\bar{1}11)$, $(1\bar{1}\bar{1})$ appears in all cubic groups and the respective scanning groups are trigonal with a rhombohedral lattice. The following abbreviated symbols are used for vectors of the cube diagonals:

$$\boldsymbol{\tau} = (\mathbf{a} + \mathbf{b} + \mathbf{c}), \quad \boldsymbol{\tau}_1 = (\mathbf{a} - \mathbf{b} - \mathbf{c}),$$
$$\boldsymbol{\tau}_2 = (-\mathbf{a} + \mathbf{b} - \mathbf{c}), \quad \boldsymbol{\tau}_3 = (-\mathbf{a} - \mathbf{b} + \mathbf{c})$$

in directions [111], $[1\bar{1}\bar{1}]$, $[\bar{1}1\bar{1}]$ and $[\bar{1}\bar{1}1]$, see Fig. 5.2.4.8. The latter three vectors are obtained from the vector $\boldsymbol{\tau}$ by the action of twofold axes as follows: $2_z\boldsymbol{\tau} = \boldsymbol{\tau}_3$, $2_x\boldsymbol{\tau} = \boldsymbol{\tau}_1$, $2_y\boldsymbol{\tau} = \boldsymbol{\tau}_2$. The rhombohedral unit cells of the scanning groups corresponding to the orientation (111) and for the P-, I- and F-centring types of original cubic groups are shown in Figs. 5.2.4.9(*a*), 5.2.4.10(*a*) and 5.2.4.11(*a*), respectively. Eight conventional cubic cells surrounding the origin are shown in each of the figures to display the hexagonal lattice in the plane corresponding to the orientation (111) and passing through the origin. The projections of these situations along the cube diagonal **d** onto this plane are depicted in Figs. 5.2.4.9(*b*), 5.2.4.10(*b*) and 5.2.4.11(*b*), respectively. In these figures, the areas that represent the choice of the hexagonal unit cell in the plane as used for scanning groups are

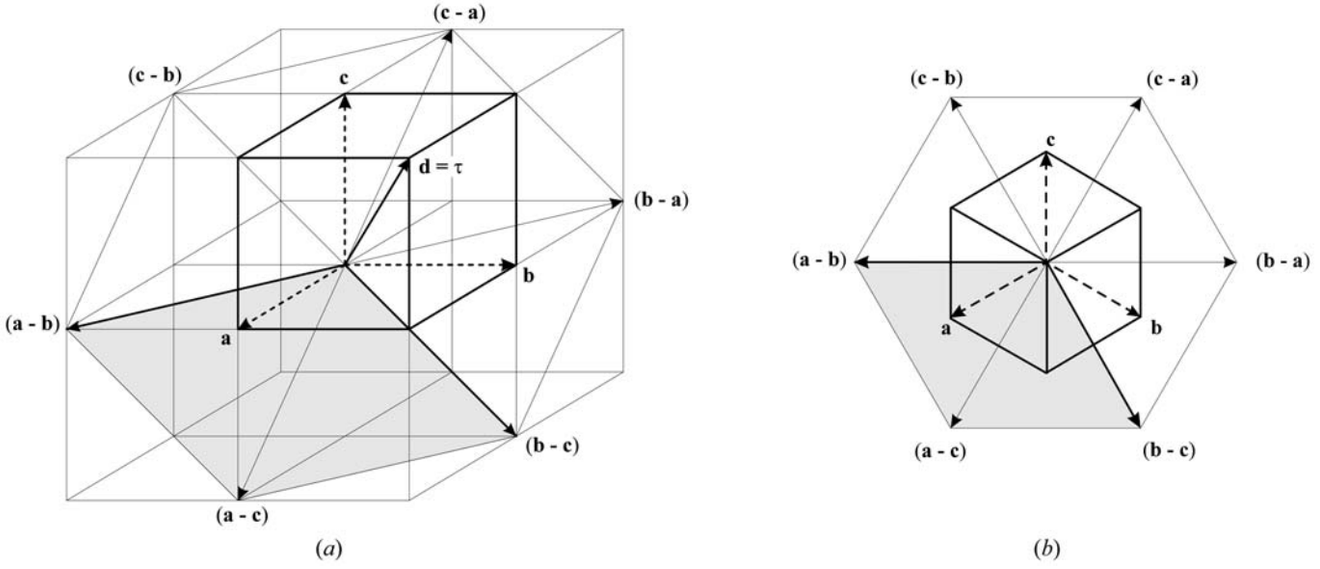

Fig. 5.2.4.9. The cubic scanning for orientation (111) in the case of cubic groups with a P lattice. (*a*) Three-dimensional view. (*b*) View along the cubic diagonal.

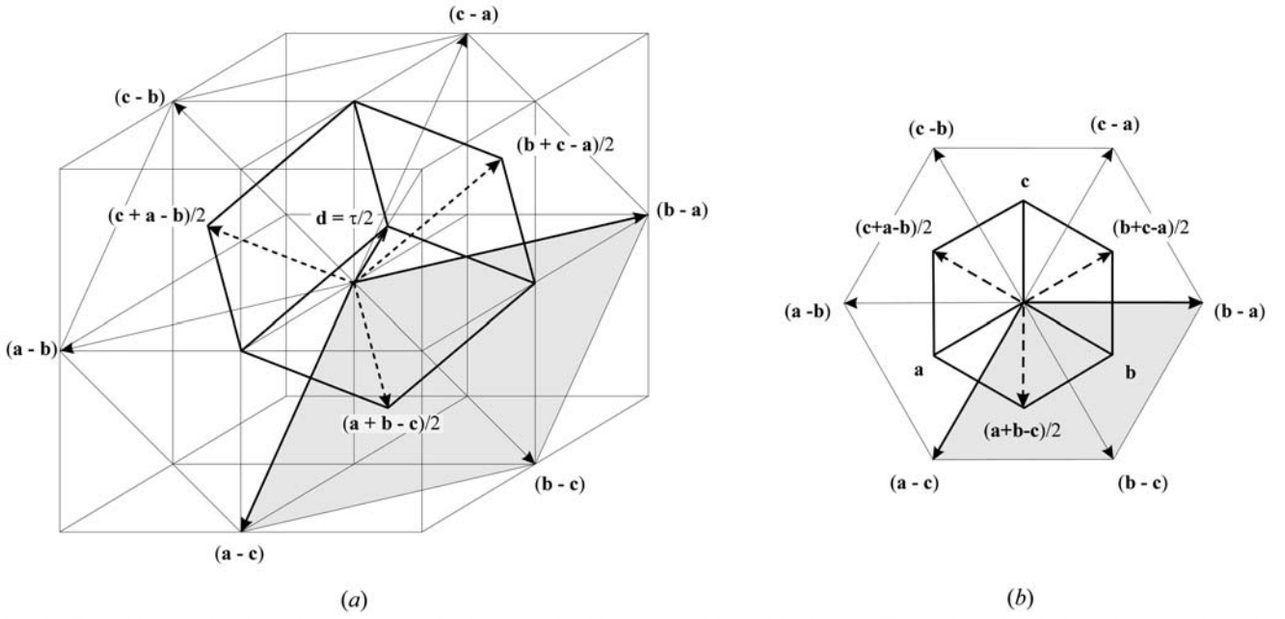

Fig. 5.2.4.10. The cubic scanning for orientation (111) in the case of cubic groups with an I lattice. (a) Three-dimensional view. (b) View along the cubic diagonal.

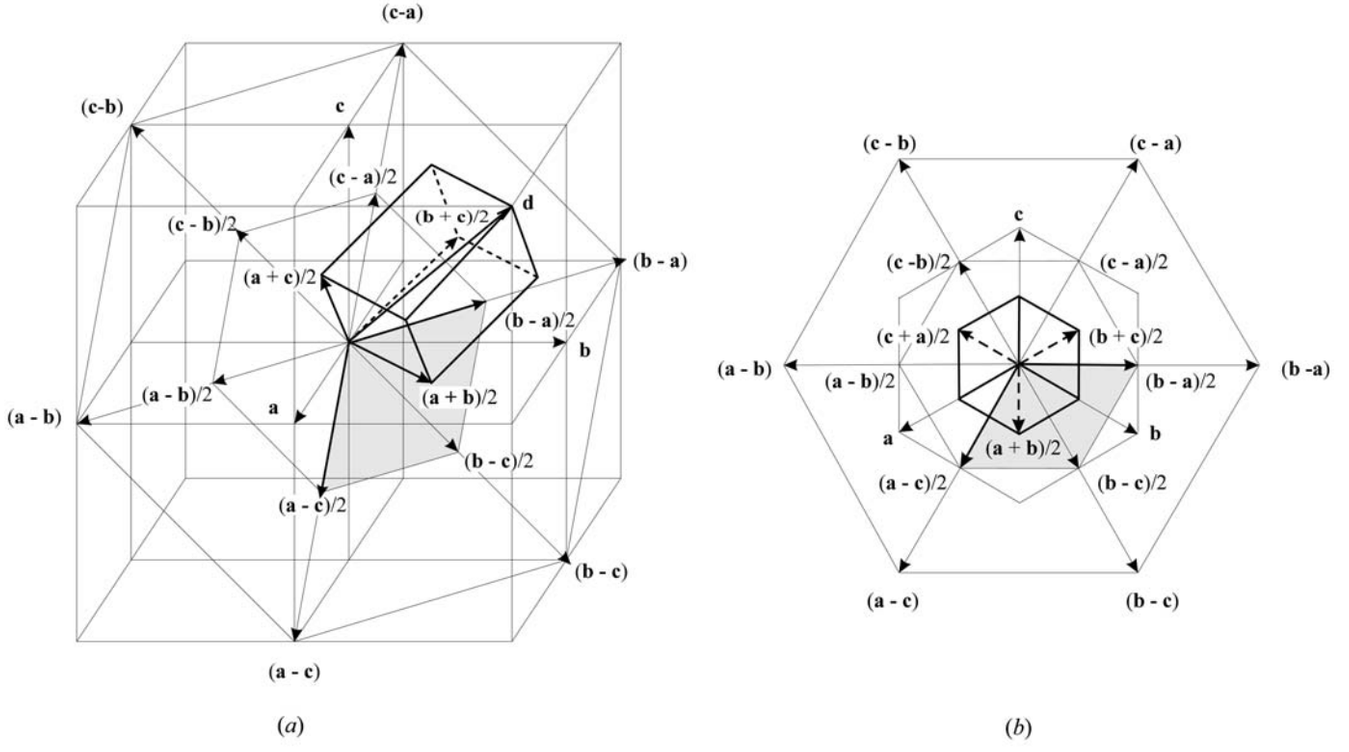

Fig. 5.2.4.11. The cubic scanning for orientation (111) in the case of cubic groups with an F lattice. (a) Three-dimensional view. (b) View along the cubic diagonal.

shaded. The scanning direction is chosen along the cube diagonal [111]. Notice that the periodicity of the corresponding hexagonal lattice in this direction equals $\mathbf{d} = \boldsymbol{\tau}$ for P- and F-centred cubic groups, while for the I-centred groups the periodicity is $\mathbf{d} = \boldsymbol{\tau}/2$. The choice of bases of the scanning groups corresponds to the obverse setting of the rhombohedral basis vectors with respect to hexagonal bases. The scanning for the direction [111] can be then copied from the scanning of trigonal groups with a rhombohedral lattice.

The remaining three orientations $(\overline{1}\overline{1}1)$, $(1\overline{1}\overline{1})$ and $(\bar{1}1\bar{1})$ are obtained by application of twofold rotations 2_z, 2_x and 2_y, respectively. Using these rotations, we obtain the scanning data in a compact way for all four orientations. Again, in certain cases, the data are the same with respect to the rotated coordinate systems; then one row describes all orientations. In other cases, the data refer to shifted coordinate systems. The shifts along the scanning direction, if they are the same for all orientations, are taken into account by recalculating the levels of the linear orbits. The shifts in planes $(\mathbf{a}', \mathbf{b}')$ are, however, used to refer to different origins.

5.2.4.6.2. *Inclined scanning, auxiliary tables*

Orientation orbit ($mn0$): Orientations of this orbit contain one of the three main cubic axes and are divided into three subsets corresponding to these axes for which the bases are separated by

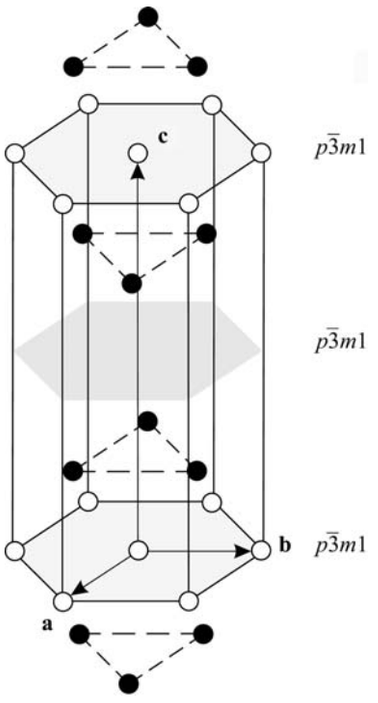

Fig. 5.2.5.1. The structure of cadmium iodide, CdI_2. The section planes of two orbits in special positions are distinguished by shading. The figure is drastically elongated in the c direction to exhibit the layer symmetries.

horizontal lines in the tables of orientation orbits and auxiliary bases. The orbit contains six orientations in groups of the Laue class $m\bar{3}$ (T_h) and 12 orientations in groups of the Laue class $m\bar{3}m$ (O_h). The orbit turns into a special orbit with fixed parameters for the special values $m = 1, n = 0$ in groups of both the Laue classes $m\bar{3}$ (T_h) and $m\bar{3}m$ (O_h). The scanning changes from monoclinic/inclined to orthorhombic in the Laue class $m\bar{3}$ (T_h), to tetragonal in the Laue class $m\bar{3}m$ (O_h). The symmetry of the orientation also increases to orthorhombic for special values $m = 1$, $n = 1$ in groups of the Laue class $m\bar{3}m$ (O_h).

The choice of bases for the three subsets is the same as in orthorhombic groups, where the orientations of subsets are separated into three different orbits and the auxiliary bases are expressed in terms of vectors of the conventional cubic basis for the centring types P and I. For the centring type F, the Miller indices differ in the original and auxiliary basis. In this case, we express the Miller indices with reference to the original basis as ($hk0$) and relate them to Miller indices ($mn0$) with reference to the auxiliary bases. These relations are the same as in the case of F-centring in orthorhombic groups, see relations (5.2.4.2) and (5.2.4.3).

Orientation orbit (*hhl*): The orbit contains 12 orientations which divide into three subsets corresponding to the three main cubic axes. In each of the subsets, one of the vectors of the conventional cubic basis is chosen as the vector $\widehat{\mathbf{b}}$ of the auxiliary basis. The orientations of the subsets are separated by horizontal lines across the table. The first subset corresponds to the vector **c** of the cubic basis and the orientations in this subset are the same as in the (*hhl*) orbit for tetragonal groups of the Laue class $4/mmm$ (D_{4h}). The orientations within each subset are further divided into two pairs of orientations to which correspond two different unique axes of the monoclinic scanning group. These subsets are again separated by horizontal lines across the last two columns. For the centring types P and I and for the first subset of orientations, the description of orientations and bases coincides with the description of the orbit (*hhl*) in tetragonal groups of the Laue class $4/mmm$ (D_{4h}) and centring types P and I, including the choice of auxiliary and conventional bases of scanning groups and relations between Miller indices h, l and m, n. For the other subsets of orientations, the data in tables are obtained by the cyclic permutation of vectors **a**, **b** and **c**.

For the centring type F, orientation (*hhl*), we choose the auxiliary basis of the scanning group with the unique axis vectors $\widehat{\mathbf{c}} = (\mathbf{a} - \mathbf{b})/2$, $\widehat{\mathbf{b}} = \mathbf{c}$ and $\widehat{\mathbf{a}} = (\mathbf{a} + \mathbf{b})/2$, while for the orientation ($h\bar{h}l$), we choose $\widehat{\mathbf{c}} = (\mathbf{a} + \mathbf{b})/2$, $\widehat{\mathbf{b}} = \mathbf{c}$ and $\widehat{\mathbf{a}} = (\mathbf{a} - \mathbf{b})/2$. The bases for the remaining orientations are again obtained by the cyclic permutation of vectors of the conventional cubic basis.

Transformation of Miller indices: The straight line in which a plane (*hhl*) intersects with the plane ($1\bar{1}0$) has the direction of a vector $(\mathbf{a} + \mathbf{b})/2h - \mathbf{c}/l$ or of the vector $\mathbf{b}' = n\widehat{\mathbf{a}} - m\mathbf{c} = n(\mathbf{a} + \mathbf{b})/2 - m\mathbf{c}$. As these two vectors can differ only by a numerical factor, the pair $(2m, n)$ must be proportional to the pair (h, l) and we obtain the relations

$$h \text{ odd } \Rightarrow m = h, n = 2l; \quad h \text{ even } \Rightarrow m = h/2, n = l,$$

recorded at the bottom row of the orientation-orbit table for the centring type F.

For the special values $h = 1, l = 0$, this orbit turns into an orbit (110) with fixed parameters and an orthorhombic scanning group.

5.2.5. Applications

5.2.5.1. *Layer symmetries in crystal structures*

The following two examples show the use of layer symmetries in the description of crystal structures.

Example 1: Fig. 5.2.5.1 shows the crystal structure of cadmium iodide, CdI_2. The space group of this crystal is $P\bar{3}m1$, D^3_{3d} (No. 164). The anions form a hexagonal close packing of spheres and the cations occupy half of the octahedral holes, filling one of the alternate layers. In close-packing notation, the CdI_2 structure is:

A	C	B	C
I	Cd	I	void

From the scanning tables, we obtain for planes with the (0001) orientation and at heights $0\mathbf{c}$ or $\frac{1}{2}\mathbf{c}$ a sectional layer symmetry $p\bar{3}m1$ (L72), and for planes of this orientation at any other height a sectional layer symmetry $p3m1$ (L69).

The plane at height $0\mathbf{c}$ contains cadmium ions. This plane defines the orbit of planes of orientation (0001) located at points $P + n\mathbf{c}$, where $n \in Z$ (Z is the set of all integers). All these planes contain cadmium ions in the same arrangement (C layer filled with Cd).

The plane at height $\frac{1}{2}\mathbf{c}$ defines the orbit of planes of orientation (0001) located at points $P + (n + \frac{1}{2})\mathbf{c}$, where $n \in Z$. All these planes lie midway between A and B layers of iodine ions with the B layer below, the A layer above the plane. They contain only voids.

The planes at levels $\frac{1}{4}\mathbf{c}$ and $\frac{3}{4}\mathbf{c}$ contain B and A layers of iodine ions, respectively. These planes and all planes produced by translations $n\mathbf{c}$ from them belong to the same orbit because the operations $\bar{3}$ exchange the A and B layers.

Example 2: The space group of cadmium chloride, $CdCl_2$, is $R\bar{3}m$, D^5_{3d} (No. 166). Fig. 5.2.5.2 shows the structure of $CdCl_2$ in its triple hexagonal cell. The anions form a cubic close packing of spheres and the cations occupy half of the octahedral holes of each alternate layer. In close-packing notation, the $CdCl_2$ structure is:

A	C	B	A	C	B	A	C	B	A	C	B
Cl	Cd	Cl	void	Cl	Cd	Cl	void	Cl	Cd	Cl	void

We choose the origin at a cadmium ion and the hexagonal basis vectors **a**, **b** as shown in Fig. 5.2.5.2. This corresponds to the obverse setting for which the scanning table is given in Part 6. The planes with the (0001) orientation at the heights $0\mathbf{c}$, $\frac{1}{6}\mathbf{c}$, $\frac{1}{3}\mathbf{c}$, $\frac{1}{2}\mathbf{c}$, $\frac{2}{3}\mathbf{c}$ and $\frac{5}{6}\mathbf{c}$ have a sectional layer group of the type $p\bar{3}m1$ (L72) and at any other height have a sectional layer group of the type $p3m1$ (L69).

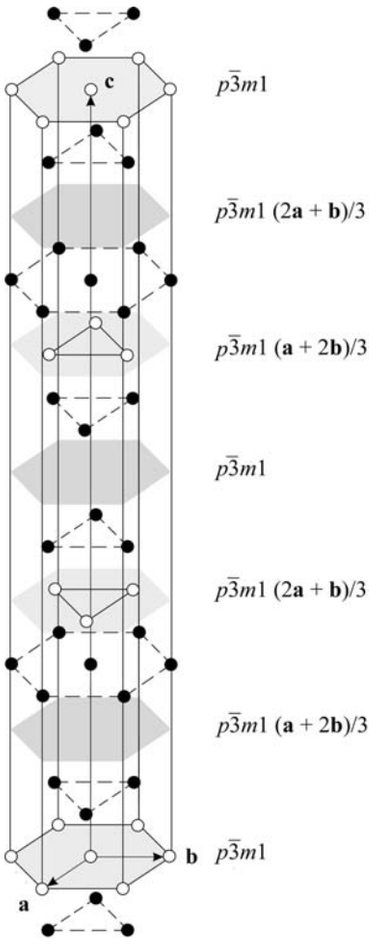

Fig. 5.2.5.2. The structure of cadmium chloride, CdI_2. The section planes of two orbits in special positions are distinguished by shading. Notice the different location of the sectional layer groups on different levels for the same orbit. The figure is drastically elongated in the *c* direction to exhibit the layer symmetries.

The scanning table also specifies the location of the sectional layer groups. The position along the *c* axis, where the basis vector $\mathbf{c} = \mathbf{d}$ specifies the scanning direction, is given by fractions of **d** or by *s***d** in the case of a general position. At the heights $0\mathbf{c}$ and $\frac{1}{2}\mathbf{c}$, the sectional layer group is the group $p\bar{3}m1$ (L72), while at the heights $\frac{1}{3}\mathbf{c}$ and $\frac{5}{6}\mathbf{c}$ it is the group $p\bar{3}m1$ $[(\mathbf{a}+2\mathbf{b})/3]$ (L72), and at the heights $\frac{2}{3}\mathbf{c}$ and $\frac{1}{6}\mathbf{c}$ it is the group $p\bar{3}m1$ $[(2\mathbf{a}+\mathbf{b})/3]$, (L72), where the vectors in brackets mean the shift of the group $p\bar{3}m1$ in space. The planes at the heights $0\mathbf{d}$, $\frac{1}{3}\mathbf{d}$ and $\frac{2}{3}\mathbf{d}$ belong to one translation orbit and the layers contain cadmium ions which are shifted relative to each other by the vectors $(\mathbf{a}+2\mathbf{b})/3$ and $(2\mathbf{a}+\mathbf{b})/3$. The planes at the heights $\frac{1}{2}\mathbf{d}$, $\frac{5}{6}\mathbf{d}$ and $\frac{1}{6}\mathbf{d}$ contain the voids and are located midway between layers of chlorine ions; they belong to another linear orbit and again are shifted relative to each other by the vectors $(\mathbf{a}+2\mathbf{b})/3$ and $(2\mathbf{a}+\mathbf{b})/3$.

5.2.5.2. *Interfaces in crystalline materials*

The scanning for the sectional layer groups is a procedure which finds applications in the theory of *bicrystals* and their *interfaces*. The first of these two terms was introduced in the study of grain boundaries (Pond & Bollmann, 1979; Pond & Vlachavas, 1983; Vlachavas, 1985; Kalonji, 1985). An *ideal bicrystal* is understood to be an aggregate of two semi-infinite crystals of identical structure, meeting at a common planar boundary called the *interface*, where one of the structures, occupying half-space on one side of the interface, is misoriented and/or displaced relative to the other structure occupying the other half-space. The word interface is a synonym for a boundary and interfaces considered here are *homophase interfaces*, in contrast with *heterophase interfaces*, where the two structures are different (Sutton & Balluffi, 1995).

An independent study of domain and twin boundaries (Janovec, 1981; Zikmund, 1984) resulted in a terminology parallel to that of the *bicrystallography*. The basic concept here is the *domain twin*, which is technically a particular case of a bicrystal. In this section, we use the terminology of bicrystals, giving the terminology of domain twins, used in the next section, parenthetically.

In both cases, the aim of the analysis is to determine the symmetry group of a bicrystal (domain twin), corresponding to a certain orientation and location of the interface (domain wall or twin boundary), which is a certain layer group.

The bicrystal (domain twin) is a conceivable real structure in space!

In the first step of the analysis, one constructs a *dichromatic complex* or *pattern* [(*unordered*) *domain pair*].

The dichromatic complex (domain pair) is not a real structure!

It is an abstract construction, a superposition of two infinite crystals which have the same structure, orientation and/or location as the two semi-infinite crystals of the bicrystal (domain twin) when extended to infinity. The two components are referred to as *black and white crystals* or *variants* (*single domain states*).

The symmetry group $\mathcal{J}$ of the dichromatic complex (domain pair) is the group of those Euclidean motions which either leave both black and white crystals (domain states) invariant or which exchange them. Planes of various orientations and locations, representing the interface, are then considered as transecting the dichromatic complex (domain pair). To each such plane there corresponds a sectional layer group $\bar{\mathsf{J}}$, the elements of which leave invariant the dichromatic pattern (domain pair) and the plane. A bicrystal (domain twin) is obtained by deleting from one side of the plane the atoms of one of the components of the dichromatic pattern (single domain states) and the atoms of the second component (single domain state) from the other side of the plane. The symmetry of the bicrystal (domain twin) is a layer group which contains those elements of the sectional layer group of the dichromatic pattern (domain pair) that satisfy one of the following two conditions:

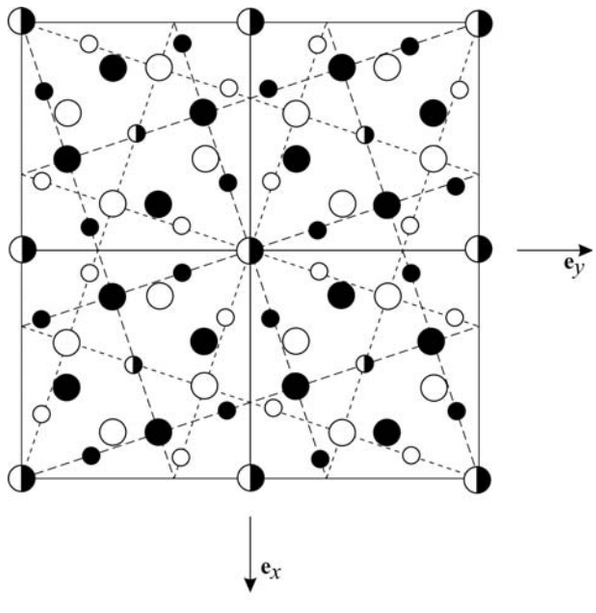

Fig. 5.2.5.3. A classical example of a bicrystal (Vlachavas, 1985).

(i) elements that leave invariant both the black and white crystals (both single domain states) and the normal to the plane;

(ii) elements that exchange the black and white crystals (single domain states) and invert the normal to the plane.

Example: Consider the bicrystal consisting of two face-centred cubic crystals misoriented by a rotation of 36.9° about the [001] direction. The corresponding dichromatic complex is shown in Fig. 5.2.5.3. The symmetry group of the complex is the space group $I4/mmm$, D_{4h}^{17} (No. 139).

Vlachavas (1985) has tabulated the symmetries of bicrystals arising when the above dichromatic complex is transected with planes of various orientations and locations. For planes of the orientation (001), given with reference to the tetragonal coordinate system shown in Fig. 5.2.5.3, Vlachavas lists

Orientation of plane	Position of plane		
(001)	$0, \frac{1}{2}$	$\frac{1}{4}, \frac{3}{4}$	Other
Symmetry group of the bicrystal	$p422$	$p42_12$	$p411$

The position of the plane is given in terms of a fraction of the basis vector of the tetragonal c axis. The 'p' in the symbol of the symmetry groups of the bicrystal denotes all translations in the (001) plane.

From the subtable for the space group $I4/mmm$, D_{4h}^{17} (No. 139) in the scanning tables, Part 6, one finds

Orientation of plane	Position of plane		
(001)	$0, \frac{1}{2}$	$\frac{1}{4}, \frac{3}{4}$	Other
Sectional layer group	$p4/mmm$	$p4/mmm$	$p4mm$

The symmetry group of the bicrystal is that subgroup of the corresponding sectional layer group consisting of all elements that satisfy one of the two conditions given above. For example, for the plane at position '0', the sectional layer group is $p4/mmm$ (L61). None of the mirror planes satisfies either of the conditions. The mirror plane perpendicular to [001] inverts the normal to the plane but leaves invariant both black and white crystals. The mirror planes perpendicular to [001] and [010] leave the normal to the plane invariant, but exchange the black and white crystals. The fourfold rotation satisfies condition (i), and the twofold rotations about auxiliary axes satisfy condition (ii). Consequently, from the sectional layer groups $p4/mmm$ (L61), $p4/nmm$ (L64) and $p4mm$ (L55) one obtains the respective symmetries of the bicrystal with different locations of interfaces: $p422$ (L53), $p42_12$ (L54) and $p4$ (L49), as listed by Vlachavas.

5.2.5.3. *The symmetry of domain twins and domain walls*

The symmetry of domain twins with planar coherent domain walls and the symmetry of domain walls themselves are also described by layer groups (see *e.g.* Janovec *et al.*, 1989), from which conclusions about the structure and tensorial properties of the domain walls can be deduced. The derivation of the layer symmetries of twins and domain walls is again facilitated by the scanning tables. As shown below, the symmetry of a twin is in general expressed through four sectional layer groups, where the central plane of the interface is considered as the section plane of an ordered and unordered domain pair. The relations between the symmetries and possible conclusions about the structure of the wall will be illustrated by an analysis of a domain twin in univalent mercurous halide (calomel) crystals.

A *twin* is a particular case of a bicrystal in which the relative orientation and/or displacement of the two components is not arbitrary; it is required that the operation that sends one of the components to the other is crystallographic. A *domain twin* is a special case where the structures S_1 and S_2 of the two components (*domains*) are distortions of a certain *parent* structure S, the symmetry of which is a certain space group $\mathcal{G}$, called the *parent group*. The parent structure S is either a real structure, the distortions of which are due to a structural phase transition, or it is a hypothetical structure. If the symmetry of one of the distorted structures S_1 is $\mathcal{F}_1$, then, from the coset decomposition

$$\mathcal{G} = \mathcal{F}_1 \cup g_2\mathcal{F}_1 \cup \ldots \cup g_p\mathcal{F}_1 \qquad (5.2.5.1)$$

we obtain $p = [\mathcal{G} : \mathcal{F}_1]$ equivalent distorted structures $\mathsf{S}_i = g_i\mathsf{S}_1$, $i = 1, 2, \ldots, p$, with symmetries $\mathcal{F}_i = g_i\mathcal{F}_1 g_i^{-1}$ which form a set of conjugate subgroups of $\mathcal{G}$.

Hence, a domain twin is always connected with a certain symmetry descent from a space group $\mathcal{G}$ to a set of conjugate subgroups $\mathcal{F}_i$. The distorted structures S_i are called the *single domain states*. A domain twin consists of two semi-infinite regions (half-spaces), called *domains*, separated by a planar interface called the *central plane*. The structures at infinite distance from this plane coincide with the domain states. The structure in the vicinity of the central plane is called the *domain wall*. The aim of the symmetry analysis is to determine the possible structure of the domain wall.

Basic theory: We consider a domain twin in which the domains are occupied by single domain states S_1 and S_2. To define the twin uniquely, we first observe that Miller indices (hkl) or corresponding normal $\mathbf{n}$ to the interface (central plane of the domain wall) define not only the orientation $V(\mathbf{a}', \mathbf{b}')$ of the wall but also its *sidedness*, so that one can distinguish between the two half-spaces. The normal $\mathbf{n}$ points from one of the half-spaces to the other while $-\mathbf{n}$ points in the opposite direction. The twin is then defined uniquely by the symbol $(\mathsf{S}_1|\mathbf{n}; s\mathbf{d}|\mathsf{S}_2) = (\mathsf{S}_1|(hkl); s\mathbf{d}|\mathsf{S}_2)$, which means that the domains are separated by the plane $(P + s\mathbf{d}; V(\mathbf{a}', \mathbf{b}'))$ of orientation $V(\mathbf{a}', \mathbf{b}')$ and location $s\mathbf{d}$, where $\mathbf{d}$ is the scanning vector. The symbol also specifies that the normal $\mathbf{n}$ points from the half-space occupied by domain state S_1 to the half-space occupied by domain state S_2.

Now we consider the changes of the twin under the action of those isometries which leave the plane $(P + s\mathbf{d}; V(\mathbf{a}', \mathbf{b}'))$ invariant. The action of such an isometry g on the twin is expressed by $g(\mathsf{S}_1|\mathbf{n}|\mathsf{S}_2) = (g\mathsf{S}_1|\widehat{g}\mathbf{n}|g\mathsf{S}_2)$, where $\widehat{g}$ is the *linear constituent* of the isometry g and $\widehat{g}\mathbf{n} = \pm\mathbf{n}$. Among these isometries, there are in general two kinds which define the symmetry of the twin and two which reverse the twin. The symbols for these four kinds of operations, their action on the initial twin $(\mathsf{S}_1|\mathbf{n}|\mathsf{S}_2)$, their graphical representation and the names of the resulting twins are as shown in Fig. 5.2.5.4.

An auxiliary notation has been introduced in which an asterisk labels operations that exchange the domain states and an underline labels operations that change the normal to the plane of the wall. To avoid misinterpretation (the symbolism is similar to that of the symmetry–antisymmetry groups), let us emphasize that neither the asterisk nor the underline have any meaning of an operation; they are just suitable labels which can be omitted without changing the meaning of general or specific symbols of the isometries. Operations with these labels mean the same as if the labels are dropped.

The operations f_{12} leave invariant the normal $\mathbf{n}$ as well as the states S_1 and S_2. Such operations are called the *trivial symmetry operations of a domain twin* and they constitute a certain layer

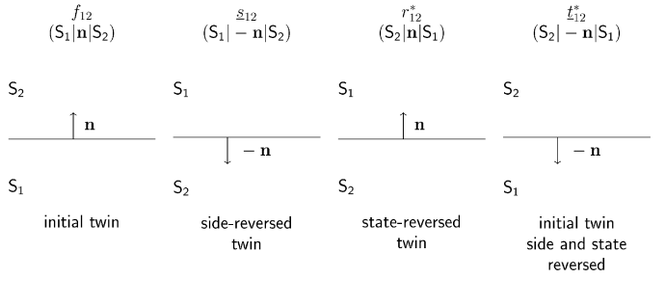

Fig. 5.2.5.4. The four types of operations on a twin.

group $\widehat{\mathsf{F}}_{12}$. The $\underline{t}^*_{12}$ exchange the half-spaces because they invert the normal **n** and at the same time they exchange the domain states S_1 and S_2. As a result they leave the twin invariant, changing only the direction of the normal. These operations are called the *non-trivial symmetry operations of a domain twin*. If $\underline{t}^*_{12}$ is one such operation, then all these operations are contained in a coset $\underline{t}^*_{12}\widehat{\mathsf{F}}_{12}$. Operations $\underline{s}_{12}$, called *the side-reversing operations*, exchange the half-spaces, leaving the domain states S_1 and S_2 invariant, and operations r^*_{12}, called *the state-reversing operations*, exchange the domain states S_1 and S_2, leaving the half-spaces invariant.

The symmetry group $\mathsf{T}(\mathsf{S}_1|\mathbf{n}; s\mathbf{d}|\mathsf{S}_2)$, or in short T_{12}, of the twin $(\mathsf{S}_1|\mathbf{n}; s\mathbf{d}|\mathsf{S}_2)$ can therefore be generally be expressed as

$$\mathsf{T}_{12} = \widehat{\mathsf{F}}_{12} \cup \underline{t}^*_{12}\widehat{\mathsf{F}}_{12}, \tag{5.2.5.2}$$

where $\widehat{\mathsf{F}}_{12}$ is a group of all trivial symmetry operations and $\underline{t}^*_{12}\widehat{\mathsf{F}}_{12}$ is the coset of all non-trivial symmetry operations of the twin.

The group T_{12} is a layer group which can be deduced from four sectional layer groups of two space groups which describe the symmetry of two kinds of domain pairs formed from the domain states S_1 and S_2 (Janovec, 1972):

An *ordered domain pair* $(\mathsf{S}_1, \mathsf{S}_2) \neq (\mathsf{S}_2, \mathsf{S}_1)$ is an analogue of the dichromatic complex in which we keep track of the two components. The symmetry group of this pair must therefore leave invariant both domain states and is expressed as the intersection

$$\mathcal{F}_{12} = \mathcal{F}_1 \cap \mathcal{F}_2 = \mathcal{F}_1 \cap g_{12}\mathcal{F}_1 g_{12}^{-1} \tag{5.2.5.3}$$

of symmetry groups $\mathcal{F}_1$ and $\mathcal{F}_2 = g_{12}\mathcal{F}_1 g_{12}^{-1}$ of the respective single domain states S_1 and S_2, where g_{12} is an operation transforming S_1 into S_2: $\mathsf{S}_2 = g_{12}\mathsf{S}_1$.

The sectional layer group $\bar{\mathsf{F}}_{12}$ of the central plane with normal **n** and at a position $s\mathbf{d}$ under the action of the space group $\mathcal{F}_{12}$ is generally expressed as

$$\bar{\mathsf{F}}_{12} = \widehat{\mathsf{F}}_{12} \cup \underline{s}_{12}\widehat{\mathsf{F}}_{12}, \tag{5.2.5.4}$$

where the halving subgroup $\widehat{\mathsf{F}}_{12}$ is the floating sectional layer group at a general position $s\mathbf{d}$. The operation $\underline{s}_{12}$ inverts the normal **n** and thus exchanges half-spaces on the left and right sides of the wall, where the left side is occupied by the state S_1 and the right side by the state S_2 in the initial twin. *These operations appear only at special positions of the central plane*. Since the half-spaces are occupied by domain states S_1 and S_2, their exchange is accompanied by an exchange of domain states on both sides of the wall. The operation $\underline{s}_{12}$ changes neither S_1 nor S_2 and hence it results in a *reversed domain twin* which has domain state S_2 on the left side and the domain state S_1 on the right side of the wall.

The *unordered domain pair* $\{\mathsf{S}_1, \mathsf{S}_2\} = \{\mathsf{S}_2, \mathsf{S}_1\}$ has the symmetry described by the group

$$\mathcal{J}_{12} = \mathcal{F}_{12} \cup j^*_{12}\mathcal{F}_{12}, \tag{5.2.5.5}$$

where j^*_{12} is an operation that exchanges S_1 and S_2, $j^*_{12}\mathsf{S}_1 = \mathsf{S}_2$, $j^*_{12}\mathsf{S}_2 = \mathsf{S}_1$. Since for an unordered domain pair $\{\mathsf{S}_1, \mathsf{S}_2\} = \{\mathsf{S}_2, \mathsf{S}_1\}$, the symmetry operations of the left coset $j^*_{12}\mathcal{F}_{12}$ are also symmetry operations of the unordered domain pair $\{\mathsf{S}_1, \mathsf{S}_2\}$. If such an operation j^*_{12} and hence the whole coset $j^*_{12}\mathcal{F}_{12}$ of state-reversing operations exists, then the domain pair is called *transposable*. Otherwise $\mathcal{J}_{12} = \mathcal{F}_{12}$ and the domain pair is called *non-transposable*.

The sectional layer group of the space group $\mathcal{J}_{12}$ can therefore be generally written in the form

$$\bar{\mathsf{J}}_{12} = \widehat{\mathsf{F}}_{12} \cup r^*_{12}\widehat{\mathsf{F}}_{12} \cup \underline{s}_{12}\widehat{\mathsf{F}}_{12} \cup \underline{t}^*_{12}\widehat{\mathsf{F}}_1. \tag{5.2.5.6}$$

In the general case, the group $\bar{\mathsf{J}}_{12}$ contains three halving subgroups which intersect at the subgroup $\widehat{\mathsf{F}}_{12}$ of index four: the subgroup $\widehat{\mathsf{J}}_{12} = \widehat{\mathsf{F}}_{12} \cup r^*_{12}\widehat{\mathsf{F}}_{12}$ is the floating subgroup of $\bar{\mathsf{J}}_{12}$; the coset $r^*_{12}\widehat{\mathsf{F}}_{12}$ is present if and only if the domain pair is transposable. The group $\bar{\mathsf{F}}_{12} = \widehat{\mathsf{F}}_{12} \cup \underline{s}_{12}\widehat{\mathsf{F}}_{12}$ is the sectional layer group for the ordered domain pair defined above. Finally, the group $\mathsf{T}_{12} = \widehat{\mathsf{F}}_{12} \cup \underline{t}^*_{12}\widehat{\mathsf{F}}_{12}$ is the symmetry group of the twin [see (5.2.5.2)]. Notice that it is itself not a sectional layer group of the space groups $\mathcal{F}_{12}$ and $\mathcal{J}_{12}$ involved unless $\mathsf{T}_{12} = \widehat{\mathsf{F}}_{12}$, which occurs in the case of a non-transposable domain pair and of a general position of the central plane.

Since the cosets can be set-theoretically expressed as differences of groups: $r^*_{12}\widehat{\mathsf{F}}_{12} = \widehat{\mathsf{J}}_{12} - \widehat{\mathsf{F}}_{12}$ and $\underline{s}_{12}\widehat{\mathsf{F}}_{12} = \bar{\mathsf{F}}_{12} - \widehat{\mathsf{F}}_{12}$, while $\mathsf{T}_{12} = \bar{\mathsf{J}}_{12} - [r^*_{12}\widehat{\mathsf{F}}_{12} \cup \underline{s}_{12}\widehat{\mathsf{F}}_{12}]$, we receive a compact set-theoretical expression for the symmetry group of the twin in terms of four sectional layer groups:

$$\mathsf{T}_{12} = \bar{\mathsf{J}}_{12} - [(\widehat{\mathsf{J}}_{12} - \widehat{\mathsf{F}}_{12}) \cup (\bar{\mathsf{F}}_{12} - \widehat{\mathsf{F}}_{12})]. \tag{5.2.5.7}$$

Thus the symmetry group T_{12} of the twin can be expressed in terms of two sectional layer groups $\bar{\mathsf{F}}_{12}$, $\bar{\mathsf{J}}_{12}$ and their floating subgroups $\widehat{\mathsf{F}}_{12}$, $\widehat{\mathsf{J}}_{12}$, respectively. These four sectional layer groups can be found in the scanning tables.

As an illustrative example, we consider below a domain twin with a ferroelastic wall in the orthorhombic ferroelastic phase of the calomel crystal Hg_2Cl_2. Original analysis which includes the domain twin with antiphase boundary is given by Janovec & Zikmund (1993). Another analysis performed prior to the scanning tables is that of the domain twin in the KSCN crystal (Janovec *et al.*, 1989). Various cases of domain twins in fullerene C_{60} have also been analysed with the use of scanning tables (Janovec & Kopský, 1997; Saint-Grégoire, Janovec & Kopský, 1997).

Example: The parent phase of calomel has a tetragonal body-centred structure of space-group symmetry $I4/mmm$ (D^{17}_{4h}), where lattice points are occupied by calomel molecules which have the form of Cl–Hg–Hg–Cl chains along the c axis. The crystallographic coordinate system is defined by vectors of the conventional tetragonal basis $\mathbf{a}_t = a\mathbf{e}_x$, $\mathbf{b}_t = a\mathbf{e}_y$, $\mathbf{c}_t = c\mathbf{e}_z$ with reference to the Cartesian basis $(\mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z)$ and the origin P is chosen at the centre of gravity of one of the calomel molecules. The parent structure projected onto the $z = 0$ plane is depicted in the middle of Fig. 5.2.5.5, where full and empty circles denote the centres of gravity at the levels $z = 0$ and $z = c/2$, respectively.

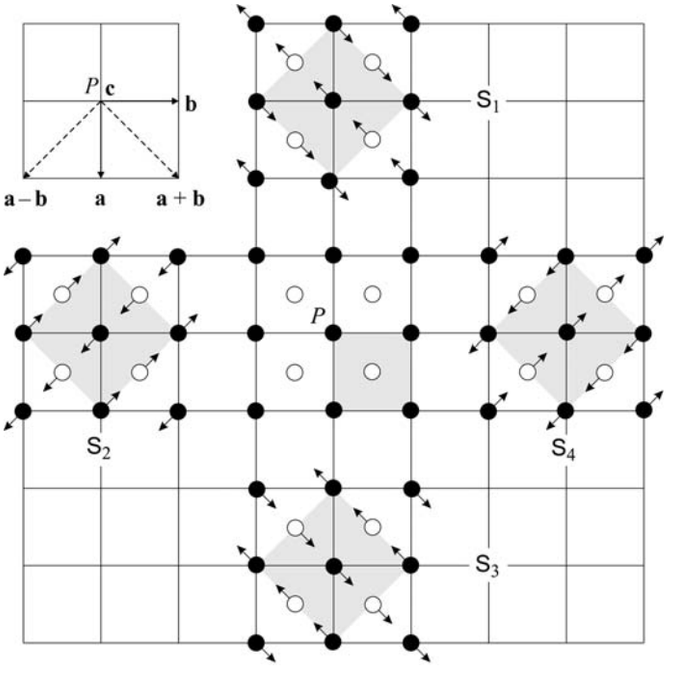

Fig. 5.2.5.5. The unit cell of the parent structure of calomel and the cells of four ferroic domain states.

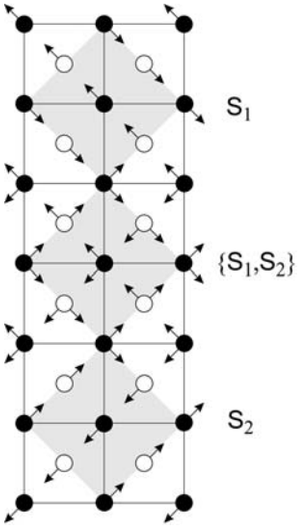

Fig. 5.2.5.6. The unordered domain pair between the two domain states.

The ferroic phase is orthorhombic with a space-group symmetry of the type *Cmcm* (D_{2h}^{17}), the conventional orthorhombic cell is based on vectors $\mathbf{a} = \mathbf{a}_t - \mathbf{b}_t$, $\mathbf{b} = \mathbf{a}_t + \mathbf{b}_t$, $\mathbf{c} = \mathbf{c}_t$ and contains two original cells. The conventional cell of the original tetragonal structure S and the cells of the four single domain states S_1, S_2, S_3 and S_4 are shaded in Fig. 5.2.5.5. The arrows represent spontaneous shifts (x, x), $(-x, x)$, $(-x, -x)$ and $(x, -x)$ of gravity centres of molecules. The two single domain states S_1 and S_3 have the symmetry *Amam* ($\mathbf{a}_t/2$ or $\mathbf{b}_t/2$); the other two single domain states S_2 and S_4 have the symmetry *Bbmm* ($\mathbf{a}_t/2$ or $\mathbf{b}_t/2$), where the Hermann–Mauguin symbols refer to the orthorhombic basis. There are two classes of domain pairs, represented by the pairs $\{\mathsf{S}_1, \mathsf{S}_2\}$ and $\{\mathsf{S}_1, \mathsf{S}_3\}$, which result in domain walls referred to as a ferroelastic domain wall and an antiphase boundary, respectively. We shall consider the first of these cases.

Table 5.2.5.1. *Symmetries of domain states and domain pairs in a calomel crystal*

All groups in this table are expressed by their Hermann–Mauguin symbols with reference to orthorhombic basis $\mathbf{a} = \mathbf{a}_t - \mathbf{b}_t$, $\mathbf{b} = \mathbf{a}_t + \mathbf{b}_t$, $\mathbf{c} = \mathbf{c}_t$.

Object	Symmetry group	Type
Parent phase	$\mathcal{G} = I4/mmm$	D_{4h}^{17}
S_1	$\mathcal{F}_1 = Am_{x\bar{y}}a_{xy}m_z$ ($\mathbf{a}_t/2$ or $\mathbf{b}_t/2$)	D_{2h}^{17}
S_2	$\mathcal{F}_2 = Bb_{x\bar{y}}m_{xy}m_z$ ($\mathbf{a}_t/2$ or $\mathbf{b}_t/2$)	D_{2h}^{17}
$(\mathsf{S}_1, \mathsf{S}_2)$	$\mathcal{F}_{12} = Pn_{x\bar{y}}n_{xy}m_z$ ($\mathbf{a}_t/2$ or $\mathbf{b}_t/2$)	D_{2h}^{12}
$\{\mathsf{S}_1, \mathsf{S}_2\}$	$\mathcal{J}_{12} = P4_{2z}^*/m_z n_{xy} m_x^*$ ($\mathbf{b}_t/2$)	D_{4h}^{14} $[D_{2h}^{12}]$

The two single domain states S_1, S_2 and the unordered pair $\{\mathsf{S}_1, \mathsf{S}_2\}$ are represented in Fig. 5.2.5.6. The symmetries of the single domain states and of both the ordered and unordered pair are given in Table 5.2.5.1, where subscripts indicate the orientation of symmetry elements with reference to the Cartesian basis and an asterisk denotes operations that exchange the single domain states.

We consider the domain walls of the orientation (100) with reference to the original tetragonal basis $(\mathbf{a}_t, \mathbf{b}_t, \mathbf{c}_t)$. This is the orientation with the Miller indices (110) with reference to the orthorhombic basis $(\mathbf{a}, \mathbf{b}, \mathbf{c})$. Consulting the scanning table No. 136 for the group $\mathcal{J}_{12} = P4_{2z}^*/m_z n_{xy} m_x^*$ ($\mathbf{b}_t/2$), we find the scanning group $Bm_y m_z m_x$ ($\mathbf{b}_t/2$) with reference to its conventional basis $(\mathbf{a}' = 2\mathbf{b}_t, \mathbf{b}' = \mathbf{c}_t, \mathbf{d} = 2\mathbf{a}_t)$, where $\mathbf{a}' = (-\mathbf{a} + \mathbf{b})$, $\mathbf{b}' = \mathbf{c}$, $\mathbf{d} = (\mathbf{a} + \mathbf{b})$. Applying the results of the scanning table with the shift by $\mathbf{b}_t/2 = \mathbf{a}'/4$, we obtain the sectional layer groups $\bar{\mathsf{J}}_{12}(0\mathbf{d})$ and $\bar{\mathsf{J}}_{12}(\frac{1}{4}\mathbf{d})$ and their floating subgroup $\bar{\mathsf{J}}_{12}(s\mathbf{d}) = \widehat{\mathsf{J}}_{12}(s\mathbf{d})$ (for $s \neq 0, \frac{1}{4}$). Analogously, for the space group $\mathcal{F}_{12}$, we obtain the sectional layer groups $\bar{\mathsf{F}}_{12}(0\mathbf{d})$ and $\bar{\mathsf{F}}_{12}(\frac{1}{4}\mathbf{d})$ and their floating subgroup $\bar{\mathsf{F}}_{12}(s\mathbf{d}) = \widehat{\mathsf{F}}_{12}(s\mathbf{d})$ (for $s \neq 0, \frac{1}{4}$). All these groups are collected in the Table 5.2.5.2 in two notations. In this table, with a specified basis, each standard symbol contains the same information as the optional symbol. Optional symbols contain subscripts which explicitly specify the orientations of symmetry elements with reference to the Cartesian coordinate system $(\mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z)$, asterisks and underlines have the meaning specified above. The lattice symbol p means the common lattice $T(2\mathbf{b}_t, \mathbf{c}_t) = T(\mathbf{a}', \mathbf{b}')$ of all sectional layer groups and twin symmetries. The Hermann–Mauguin symbols are written with reference to the coordinate systems $(P + s\mathbf{d}; \mathbf{a}', \mathbf{b}', \mathbf{d})$.

The twin symmetry $\mathsf{T}_{12}(s\mathbf{d})$ is determined by the relation (5.2.5.7). This means, in practice, that we have to find the groups $\bar{\mathsf{J}}_{12}(s\mathbf{d})$, $\widehat{\mathsf{J}}_{12}(s\mathbf{d})$, $\bar{\mathsf{F}}_{12}(s\mathbf{d})$ and $\widehat{\mathsf{F}}_{12}(s\mathbf{d})$ from which we obtain the group $\mathsf{T}_{12}(s\mathbf{d})$. If tables of subgroups of layer groups were available, it would be sufficient to look up the subgroups which lie between $\bar{\mathsf{J}}_{12}(s\mathbf{d})$ and $\widehat{\mathsf{F}}_{12}(s\mathbf{d})$ and recognize the three groups $\bar{\mathsf{F}}_{12}(s\mathbf{d})$, $\widehat{\mathsf{J}}_{12}(s\mathbf{d})$ and $\mathsf{T}_{12}(s\mathbf{d})$.

Optional symbols facilitate this determination considerably. To get the twin symmetry $\mathsf{T}_{12}(s\mathbf{d})$, we look up the optional symbol for the group $\bar{\mathsf{J}}_{12}(s\mathbf{d})$ and eliminate elements that are either only underlined or that are only labelled by an asterisk. Or, *vice versa*, we leave only those elements that are not labelled at all or that are at the same time underlined and labelled by an asterisk. The resulting twin symmetries are given in the lower part of Table 5.2.5.2.

The implications of this symmetry analysis on the structure of domain walls at $0\mathbf{d}$ and $\frac{1}{4}\mathbf{d}$ are illustrated in Fig. 5.2.5.7. Shaded areas represent the domain states at infinity. The left-hand part of

Table 5.2.5.2. *Sectional layer groups of space groups $\mathcal{F}_{12}$ and $\mathcal{J}_{12}$ in the conventional basis $(\mathbf{a}' = 2\mathbf{b}_t, \mathbf{b}' = \mathbf{c}_t, \mathbf{d} = 2\mathbf{a}_t)$ of the scanning group $Bm_y m_z m_x$ and the respective twin symmetries*

Space group	Plane (*hkl*)	Location	Sectional layer group		
		$s\mathbf{d}$	$\mathcal{L}(s\mathbf{d})$	Standard symbol	Optional symbol
$\mathcal{F}_{12}$	(110)	$0\mathbf{d}$	$\bar{\mathsf{F}}_{12}(0\mathbf{d})$	$p12/m1$ ($\mathbf{b}_t/2$)	$p1\underline{2}_z/m_z1$ ($\mathbf{b}_t/2$)
		$\frac{1}{4}\mathbf{d}$	$\bar{\mathsf{F}}_{12}(\frac{1}{4}\mathbf{d})$	$p12/m1$	$p1\underline{2}_z/m_z1$
		$s\mathbf{d}$	$\bar{\mathsf{F}}_{12}(s\mathbf{d}) = \widehat{\mathsf{F}}_{12}$	$p1m1$	$p1m_z1$
$\mathcal{J}_{12}$		$0\mathbf{d}$	$\bar{\mathsf{J}}_{12}(0\mathbf{d})$	$pmmm$ ($\mathbf{b}_t/2$)	$p2_y^*/m_y^*\ \underline{2}_z/m_z\ 2_x^*/\underline{m}_x^*$ ($\mathbf{b}_t/2$)
		$\frac{1}{4}\mathbf{d}$	$\bar{\mathsf{J}}_{12}(\frac{1}{4}\mathbf{d})$	$pmma$	$p\underline{2}_{1y}^*/m_y^*\ \underline{2}_z/m_z\ 2_x^*/\underline{a}_x^*$
		$s\mathbf{d}$	$\bar{\mathsf{J}}_{12}(s\mathbf{d}) = \widehat{\mathcal{J}}_{12}$	$pmm2$	$pm_y^*m_z2_x^*$
Twin symmetries		Location	$\mathsf{T}_{12}(s\mathbf{d})$	Symmetry of the twin	
		$0\mathbf{d}$	$\mathsf{T}_{12}(0\mathbf{d})$	$p2mm$	$p\underline{2}_y^*m_z\underline{m}_x^*$
		$\frac{1}{4}\mathbf{d}$	$\mathsf{T}_{12}(\frac{1}{4}\mathbf{d})$	$p2_1ma$	$p\underline{2}_{1y}^*m_z\underline{a}_x^*$
		$s\mathbf{d}$	$\mathsf{T}_{12}(s\mathbf{d})$	$p1m1$	$p1m_z1$

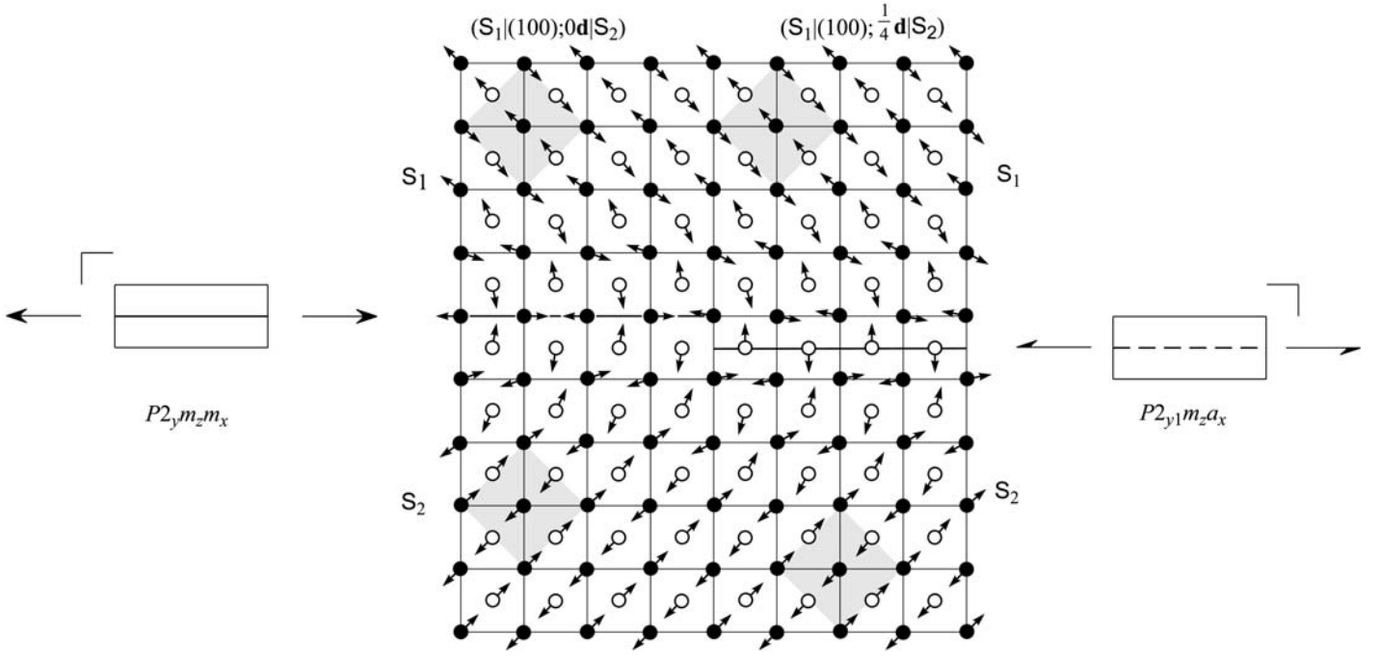

Fig. 5.2.5.7. The structures and symmetries of domain twins in calomel corresponding to two different special positions of the wall.

the figure corresponds to the location of the central plane at $0\mathbf{d}$, the right-hand part to the location at $\frac{1}{4}\mathbf{d}$. The twin symmetries $\mathsf{T}_{12}(0\mathbf{d}) = p2_y m_z m_x$ and $\mathsf{T}_{12}(\frac{1}{4}\mathbf{d}) = p2_{1y} m_z a_x$ determine the relationship between the structures in the two half-spaces. The trivial symmetry operations form the layer group $p1m_z1$ in both cases and leave invariant the structures in both half-spaces. The non-trivial symmetry operations map the structure in one of the half-spaces onto the structure in the other half-space and back. The symmetry of the central plane is given by the groups $\bar{\mathsf{J}}_{12}(0\mathbf{d})$ and $\bar{\mathsf{J}}_{12}(\frac{1}{4}\mathbf{d})$ because the states S_1 and S_2 meet at this plane.

The arrows that represent the shift of calomel molecules in the *xy* plane may rotate and change their amplitude as we approach the central plane because the symmetry requirements are relaxed to those imposed by the layer group $p1m_z1$ consisting of trivial symmetry operations of the twin. The non-trivial twin symmetries determine the relationship between the structures in the two half-spaces, so that the rotation and change of amplitude in these two half-spaces are correlated. The symmetry of the central plane requires, in the left-hand part of the figure, that the arrows at black circles are aligned along the plane and that they are of the same lengths and alternating direction. The arrows at the empty circles in the right-hand part of the figure are nearly perpendicular to the plane, of the same lengths and of alternating direction in accordance with the central-plane symmetry. They are shown in the figure as strictly perpendicular to the plane; however, slight shifts of the atoms parallel to the plane can be expected because the arrows mean that the atoms are actually already out of the central plane.

Summary: In the analysis of domain twins, we know the structures of the two domain states, in our case the orientation of arrows, at infinity. In the example above, we considered two cases in both of which the layer group $\bar{\mathsf{J}}_{12}(s_o\mathbf{d})$ contains all four types of the twin operations – two types of symmetry operations and two types of twin-reversing operations. In this case, we summarize the results of the symmetry analysis as follows. (i) The floating layer group $\widehat{\mathsf{F}}_{12}$ determines the allowed changes of the structures on the path from infinity (physically this means the domain bulk) towards the central plane. (ii) Operations of the coset $t^*_{12}\widehat{F}_{12}$ correlate the changes in the two half-spaces. (iii) The group $\bar{\mathsf{J}}_{12}(s_o\mathbf{d})$ as the symmetry of the central plane where the two half-spaces meet contains the twin symmetry $\mathsf{T}_{12}(s_o\mathbf{d})$ as its halving subgroup and therefore imposes additional conditions on the structure of the central plane in comparison with the conditions in its vicinity.

As always, the symmetry determines only the character of possible changes but neither their magnitude nor their dependence on the distance from the central plane. Thus, in the example considered, the symmetry arguments cannot predict the detailed dependence of the angle of rotation on the distance from the wall and they cannot predict whether and how the lengths of these arrows change.

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