meters 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 nontrivial 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 nontrivial 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.

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 $\mathbf{d} = \mathbf{b}$.

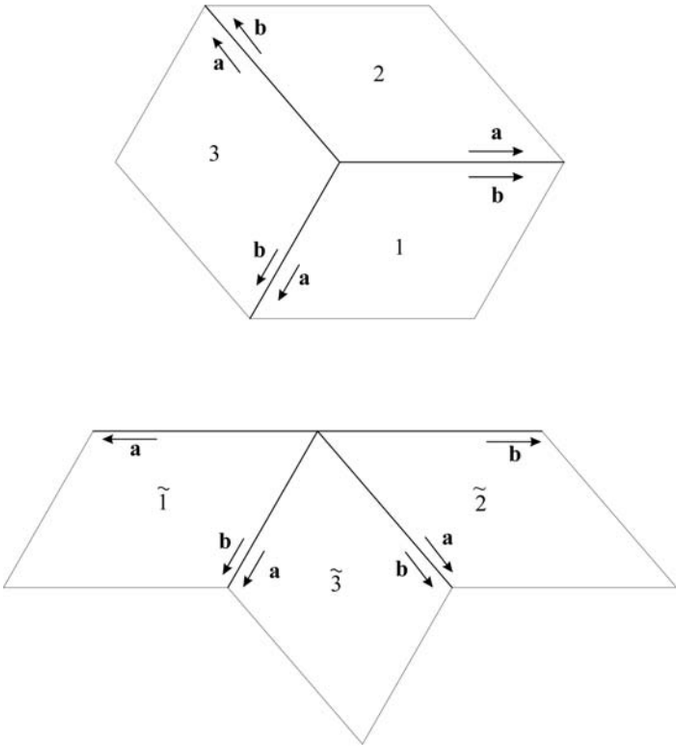

Fig. 5.2.4.1. Six monoclinic cell choices.

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 (*hk*0) 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 (*hk*0) with respect to the conventional basis (**a**, **b**, **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 (*hk*0) 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

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

so

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

and conversely

$$n = h + k, \quad m = k - h. \qquad (5.2.4.3)$$

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 **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 (**a**′, **b**′, **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), 4*mm* (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), 4*mm* (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 (110) 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 (*mn*0) occur in groups of both tetragonal Laue classes 4/*m* (C_{4h}) and 4/*mmm* (D_{4h}). Orientation orbits (0*mn*) occur only in groups of the Laue class 4/*mmm* (D_{4h}).

Orientation orbits (*mn*0): These orbits contain two orientations, namely (*mn*0) and ($\bar{n}m$0) 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 (*mn*0), ($\bar{n}m$0), ($\bar{m}n$0) and (*nm*0) in groups of the geometric classes 422 (D_4), 4*mm* (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 (*mn*0). 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 (*mn*0).

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 (0*mn*): These orbits, consisting of orientations (0*mn*), (0$\bar{m}n$), (*m*0*n*) and (*m*0$\bar{n}$), appear only in groups of the Laue class 4/*mmm* (D_{4h}). The first two orientations contain the vector **a**, the other two contain the vector **b**, scanning groups are monoclinic with unique axes along vectors **a** and **b**, respectively, for the first and second pair of orientations; the scanning is inclined because the vectors **a** and **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*), ($\overline{h}\overline{h}l$), ($h\bar{h}l$) 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

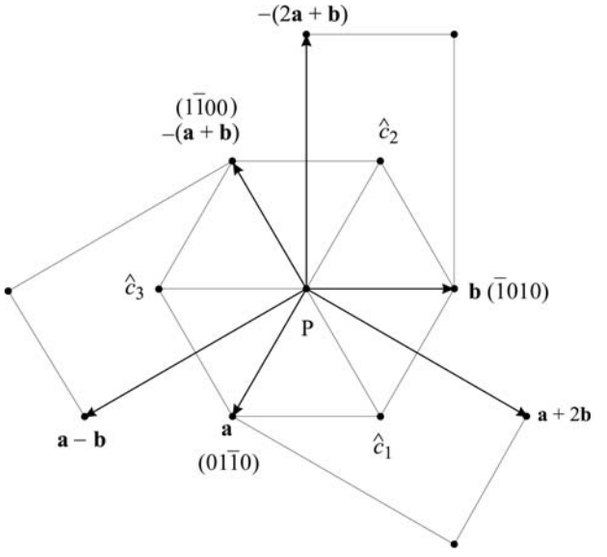

Fig. 5.2.4.2. Symbols for a hexagonal lattice with a rectangular point group.

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

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

for the first pair of orientations and as

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

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

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

for the first pair of orientations and as

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

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

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

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

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

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

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

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 nontrivial orientation orbits in groups of

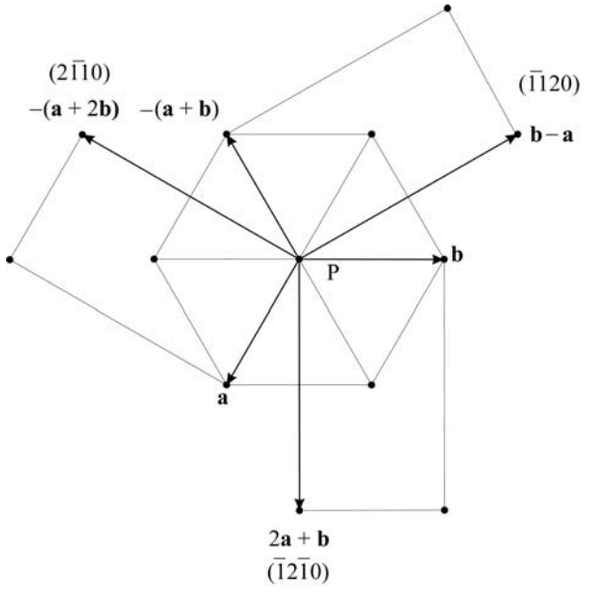

Fig. 5.2.4.3. Another choice of orthogonal basis vectors for a hexagonal lattice.

the Laue class $\bar{3}$ (C_{3i}) and no other orbits with fixed parameters in groups of the Laue class $6/m$ (C_{6h}).

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 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 **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 **b**′, **d** of one of them are replaced by −**d**, **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.

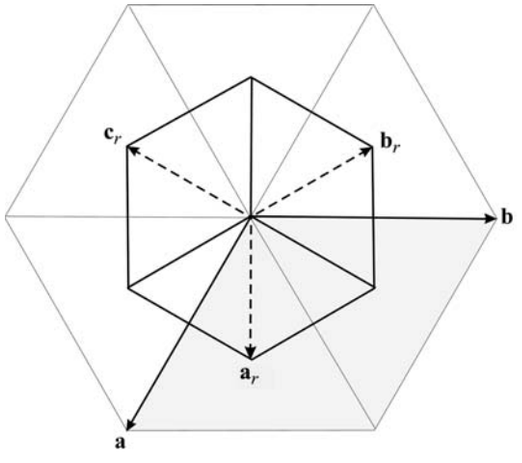

Fig. 5.2.4.4. The relationship between hexagonal and rhombohedral bases in the obverse setting.

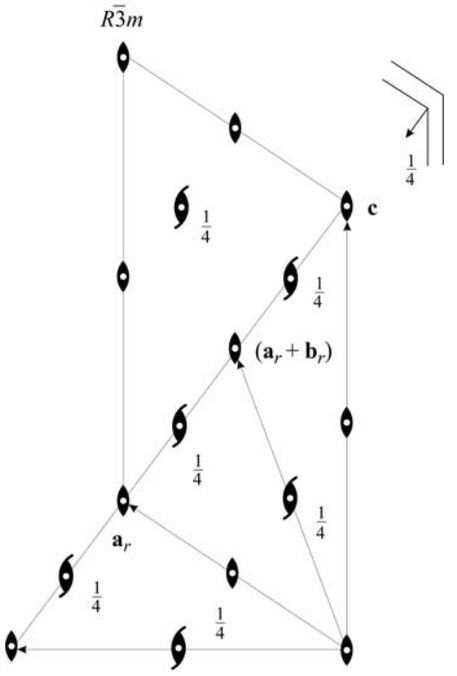

Fig. 5.2.4.5. The diagram of the scanning group $R\bar{3}m$ in the plane of orientation ($\bar{1}$2$\bar{1}$0) projected orthogonally along **b**.

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^5_{3d} (No. 166) and $R\bar{3}c$, D^6_{3d} (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

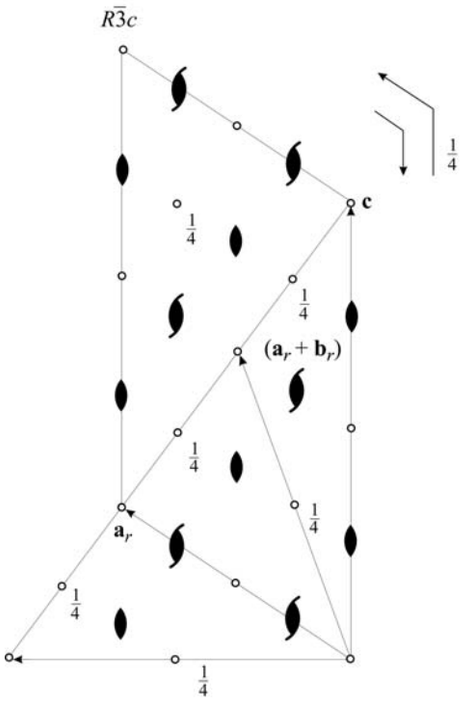

Fig. 5.2.4.6. The diagram of the scanning group $R\bar{3}c$ in the plane of orientation $(\bar{1}2\bar{1}0)$ projected orthogonally along **b**.

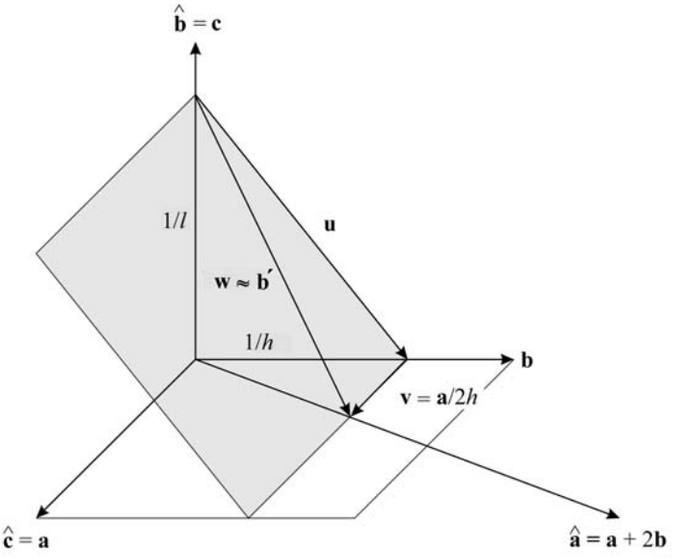

Fig. 5.2.4.7. Illustration of the transformation of Bravais–Miller indices in a hexagonal basis to Bravais indices in an auxiliary basis.

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

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

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 $(\hat{\mathbf{a}}, \hat{\mathbf{b}}, \hat{\mathbf{c}})$, 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 $\mathbf{b}' = n\hat{\mathbf{a}} - m\hat{\mathbf{b}}$, where $\hat{\mathbf{a}} = \mathbf{a} + 2\mathbf{b}$ for both the centring types P and R, while $\hat{\mathbf{b}} = \mathbf{c}$ for the centring type P and $\hat{\mathbf{b}} = \mathbf{c}_r$ 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:

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

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 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 $\mathbf{a}\rightarrow\mathbf{b}\rightarrow\mathbf{c}\rightarrow\mathbf{a}$ and $\mathbf{a}\rightarrow\mathbf{c}\rightarrow\mathbf{b}\rightarrow\mathbf{a}$, 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 (110) 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 $\mathbf{a}\rightarrow\mathbf{b}\rightarrow\mathbf{c}\rightarrow\mathbf{a}$ and the bases of scanning groups for the orientations (101) and $(\bar{1}01)$ by the cyclic permutation $\mathbf{a}\rightarrow\mathbf{c}\rightarrow\mathbf{b}\rightarrow\mathbf{a}$, 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), $(\bar{1}\bar{1}1)$, $(1\bar{1}\bar{1})$ 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 $\mathbf{d}$ onto this plane are

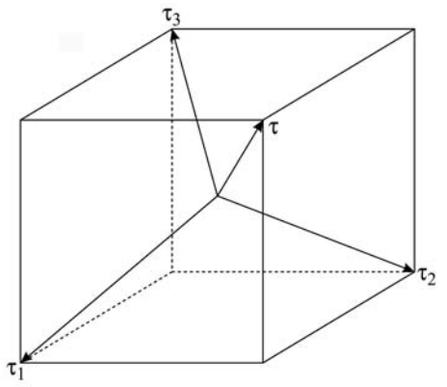

Fig. 5.2.4.8. Vectors along the main cubic axes.

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 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,

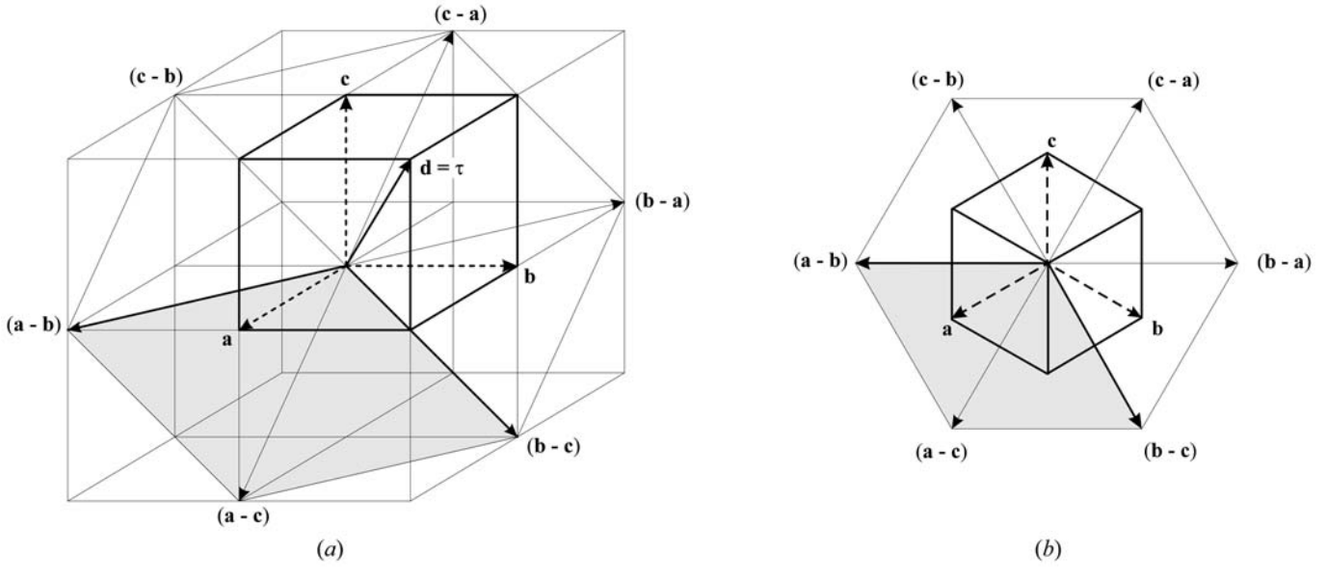

Fig. 5.2.4.9. The cubic scanning for orientation (111) in the case of cubic groups with a *P* lattice. (*a*) Three-dimensional view. (*b*) View along the cubic diagonal.

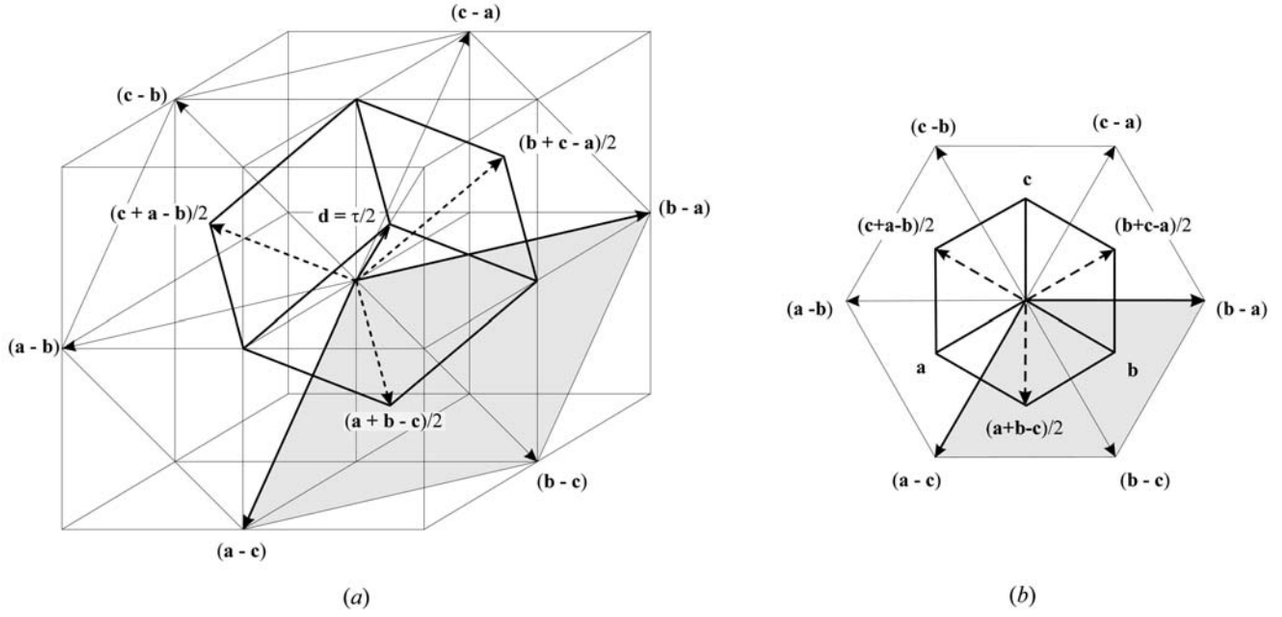

Fig. 5.2.4.10. The cubic scanning for orientation (111) in the case of cubic groups with an *I* lattice. (*a*) Three-dimensional view. (*b*) View along the cubic diagonal.

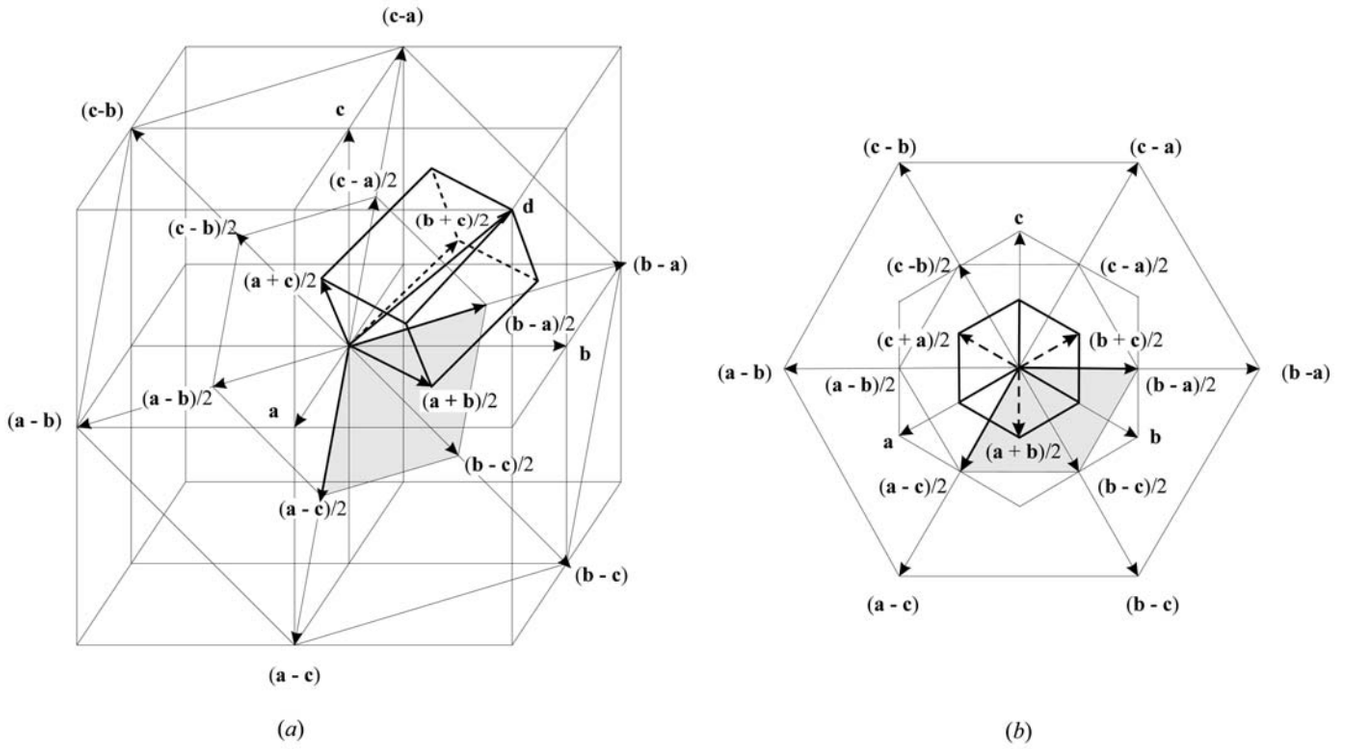

Fig. 5.2.4.11. The cubic scanning for orientation (111) in the case of cubic groups with an *F* lattice. (*a*) Three-dimensional view. (*b*) View along the cubic diagonal.

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 (*mn*0): 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 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 (*hk*0) and relate them to Miller indices (*mn*0) 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 $\mathbf{a}$, $\mathbf{b}$ 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).

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 $\mathbf{d}$ or by $s\mathbf{d}$ 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 $(2\mathbf{a} + \mathbf{b})/3$.

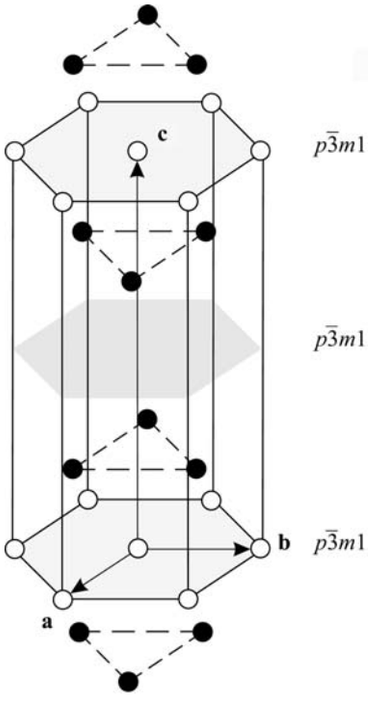

Fig. 5.2.5.1. The structure of cadmium iodide, CdI_2. The section planes of two orbits in special positions are distinguished by shading. The figure is drastically elongated in the c direction to exhibit the layer symmetries.

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.

references