5. SCANNING OF SPACE GROUPS
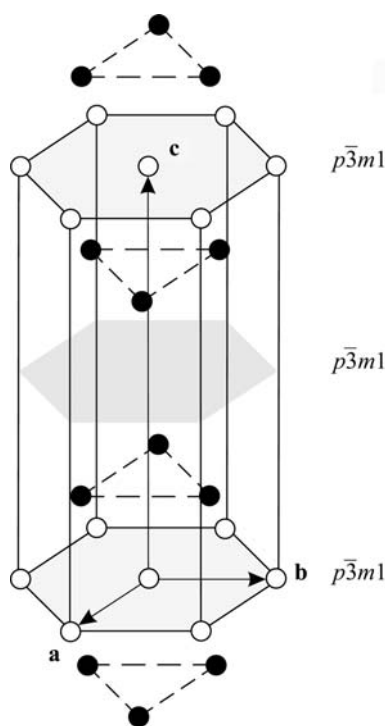

Fig. 5.2.5.1. The structure of cadmium iodide, CdI$_2$. The section planes of two orbits in special positions are distinguished by shading. The figure is drastically elongated in the c direction to exhibit the layer symmetries.

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 $\mathbf{c}$ 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 $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{c}$.

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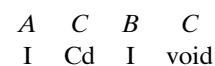
From the scanning tables, we obtain for planes with the (0001) orientation and at heights $0\mathbf{c}$ or $\frac{1}{2}\mathbf{c}$ a sectional layer symmetry $p\bar{3}m1$ (L72), and for planes of this orientation at any other height a sectional layer symmetry $p3m1$ (L69).

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_{3d}^5 (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
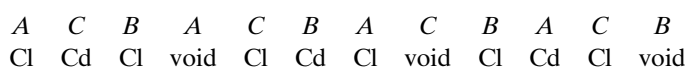
We choose the origin at a cadmium ion and the hexagonal basis vectors $\mathbf{a}$, $\mathbf{b}$ as shown in Fig. 5.2.5.2. This corresponds to the obverse setting for which the scanning table is given in Part 6. The planes with the (0001) orientation at the heights $0\mathbf{c}$, $\frac{1}{6}\mathbf{c}$, $\frac{1}{3}\mathbf{c}$, $\frac{1}{2}\mathbf{c}$, $\frac{2}{3}\mathbf{c}$ 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).
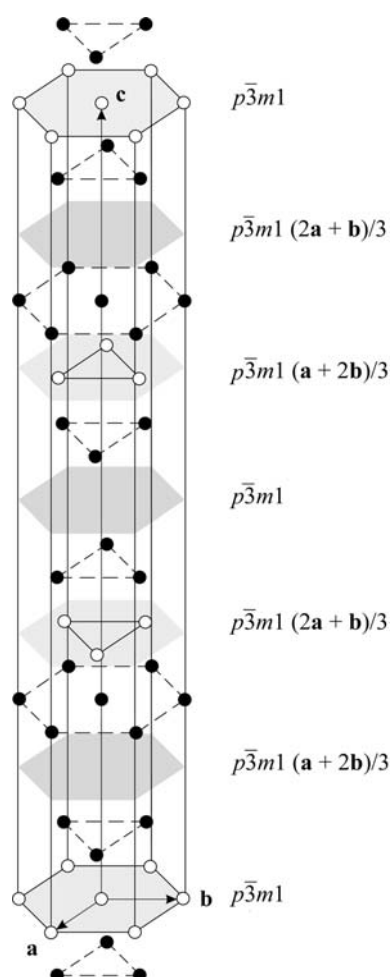
Fig. 5.2.5.2. The structure of cadmium chloride, CdI$_2$. The section planes of two orbits in special positions are distinguished by shading. Notice the different location of the sectional layer groups on different levels for the same orbit. The figure is drastically elongated in the c direction to exhibit 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 $\mathbf{d}$ 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 $(2\mathbf{a} + \mathbf{b})/3$.

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 $\underline{\mathbf{J}}$, 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:
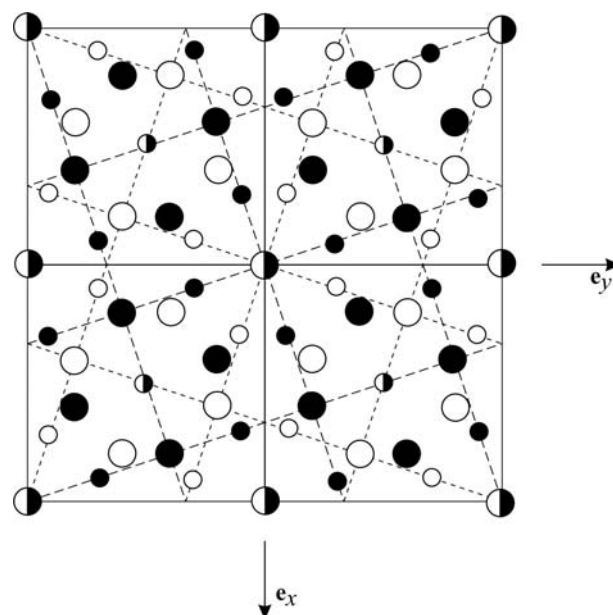

Fig. 5.2.5.3. A classical example of a bicrystal (Vlachavas, 1985).

references