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, 2005). 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 *et al.*, 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.

5.2.2. The basic concepts of the scanning

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

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

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

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

5.2.2.1. The scanning for sectional layer groups

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

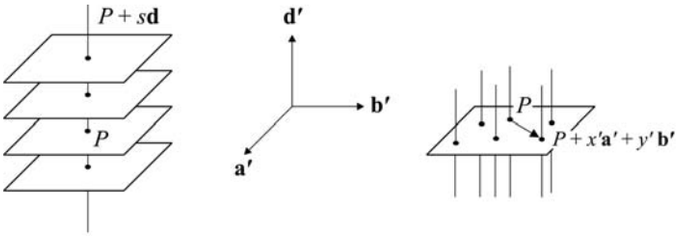

Fig. 5.2.2.1. Sets of parallel planes (left) and sets of parallel straight lines (right).

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

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

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

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

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

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

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

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