

3.4. LATTICE COMPLEXES

are $4mm$ or 4 and $\bar{4}2m$ (site symmetry m) or $\bar{4}$, respectively. The crystal form 'tetragonal prism' is a limiting form of both crystal forms 'tetragonal pyramid' and 'tetragonal disphenoid'.

If a first lattice complex forms a true subset of a second one, *i.e.* if each point configuration of the first lattice complex also belongs to the second one, then the first one is called a *limiting complex* of the second one and the second complex is called a *comprehensive complex* of the first one (*cf.* Koch & Fischer, 1985).

Example

The cubic lattice complex $I\bar{4}3d$ $16c$ x, x, x involves two limiting complexes, namely $Im\bar{3}m$ $2a$ $0, 0, 0$ and $Ia\bar{3}d$ $16b$ $\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$. The orbits from $I\bar{4}3d$ $16c$ with $x = 0$ and from $Im\bar{3}m$ $2a$ are configuration equivalent, and so are the orbits from $I\bar{4}3d$ $16c$ with $x = \frac{1}{8}$ and from $Ia\bar{3}d$ $16b$.

Example

The tetragonal lattice complex $I4_1/amd$ $4a$ is a comprehensive complex of the cubic complex $Fd\bar{3}m$ $8a$. Each orbit of $Fd\bar{3}m$ $8a$ is configuration equivalent to a crystallographic orbit of a special space group of type $I4_1/amd$ with axial ratio $c/a = (2)^{1/2}$.

Furthermore, two lattice complexes without a limiting-complex relationship may have a non-empty intersection. Then the point configurations of the intersection result in one or, in very exceptional cases, in two or more other lattice complexes (*cf.* Koch, 1974).

Example

The intersection of the two lattice complexes $Im\bar{3}$ $24g$ and $I\bar{4}3m$ $24g$ consists of all point configurations belonging to $Im\bar{3}m$ $24h$, *i.e.* each point configuration out of this intersection refers to an orbit from $Im\bar{3}m$ $24h$ $0, x, x$ and, in addition, to an orbit from $Im\bar{3}$ $24g$ $0, y, z$ with $y = z$ and to another one from $I\bar{4}3m$ $24g$ x, x, z with $z = 0$.

Example

The intersection of the trivariant lattice complexes $Fm\bar{3}c$ $192j$ and $P432$ $24k$ consists of two bivariant limiting complexes, namely of $Pm\bar{3}m$ $24k$ $0, y, z$ and of $Pm\bar{3}m$ $24m$ x, x, z .

Each point configuration of a given lattice complex is uniquely related to two space groups: (1) the space group that reflects its eigensymmetry, and (2) a space group that belongs to the characteristic space-group type of the lattice complex under consideration. In most cases the two groups coincide. Only when the point configuration under consideration belongs to a limiting complex is the first group a proper supergroup of the second one.

Complete lists of the limiting complexes of all lattice complexes are not available. Koch (1974) derived the limiting complexes of the cubic lattice complexes. The limiting complexes that refer to specialized coordinate parameters may be derived from a table by Engel *et al.* (1984), who listed the respective non-characteristic orbits for all space-group types. The limiting complexes of the tetragonal and trigonal lattice complexes that are due to metrical specializations are tabulated by Koch & Fischer (2003) and by Koch & Sowa (2005), respectively.

Fischer & Koch (1978) tabulated the limiting complexes for the crystallographic point groups, rod groups and layer groups. As each type of plane group uniquely corresponds to a certain type of isomorphic layer group, information on the limiting complexes of the lattice complexes of the plane groups may easily be extracted from the respective table for the layer

groups. This information may also be taken from a list of the non-characteristic orbits of the plane groups by Matsumoto & Wondratschek (1987).

3.4.1.5. Additional properties of lattice complexes*3.4.1.5.1. The degrees of freedom*

Each Wyckoff position shows a certain number of coordinate parameters that can be varied independently. For most lattice complexes, this number is the same for any of its Wyckoff positions. For the lattice complex with characteristic Wyckoff position $Pm\bar{3}$ $12j$ $m.. 0, y, z$, for instance, this number is two. The lattice complex has two degrees of freedom. If, however, the variation of a certain coordinate corresponds to a shift of the point configuration as a whole, the lattice complex has fewer degrees of freedom than the Wyckoff position that is being considered. Therefore, $I4_1$ $8b$ x, y, z is the characteristic Wyckoff position of a lattice complex with only two degrees of freedom, although position $8b$ itself has three coordinate parameters that can be varied independently. The lattice complex $P4/m$ j has two degrees of freedom and refers to Wyckoff positions with two as well as with three independent coordinate parameters, namely to $P4/m$ $4j$ $m.. x, y, 0$ and to $P4$ $4d$ 1 x, y, z .

According to its number of degrees of freedom, a lattice complex is called *invariant*, *univariant*, *bivariant* or *trivariant*. In total, there exist 402 lattice complexes, 36 of which are invariant, 106 univariant, 105 bivariant and 155 trivariant. The 30 plane lattice complexes are made up of 7 invariant, 10 univariant and 13 bivariant ones.

Most of the invariant and univariant lattice complexes correspond to several types of Wyckoff set. In contrast to that, only one type of Wyckoff set can belong to each trivariant lattice complex. A bivariant lattice complex may either correspond to one type of Wyckoff set (*e.g.* $Pm\bar{3}$ j) or to two types ($P4$ d , for example, belongs to the lattice complex with the characteristic Wyckoff position $P4/m$ j).

3.4.1.5.2. Weissenberg complexes

Depending on their site-symmetry groups, two kinds of Wyckoff position may be distinguished:

- (i) The site-symmetry group of any point is a proper subgroup of another site-symmetry group from the same space group. Then the Wyckoff position contains, among others, orbits where suitably chosen points may be infinitely close together.

Example

Each point configuration of the lattice complex with the characteristic Wyckoff position $P4/mmm$ $4j$ $m.2m$ $x, x, 0$ may be imagined as squares of four points surrounding the points of a tetragonal primitive lattice. For $x \rightarrow 0$, the squares become infinitesimally small. Orbits with $x = 0$ show site symmetry $4/mmm$, their multiplicity is decreased from 4 to 1, and they belong to Wyckoff position $P4/mmm$ $1a$.

- (ii) The site-symmetry group of every point belonging to the Wyckoff position under consideration is not a proper subgroup of any other site-symmetry group from the same space group.

Example

In $Pmma$, there does not exist a site-symmetry group that is a proper supergroup of $mm2$, the site symmetry of Wyckoff position $Pmma$ $2e$ $\frac{1}{4}, 0, z$. As a consequence, the