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point configurations may be derived as described above, but now – instead of starting from just a particular group – starting from all space groups of type $P4/mmm$ with all conceivable positions of the origins and lengths and orientations of the basis vectors. Accordingly, the point configurations may differ in their relative position in space, their orientation, and in the distances between the centres and the size of their squares.

Just as all crystal forms of a particular type may be related to different point-group types, the same lattice complex may occur in different space-group types.

Example

The lattice complex 'cubic primitive lattice' may be generated, among others, in $Pm\bar{3}m$ $1a, b$, in $Fm\bar{3}m$ $8c$ and in $Ia\bar{3}$ $8a, b$ with site symmetry $m\bar{3}m$, $\bar{4}3m$ and $.\bar{3}.$, respectively. The type of Wyckoff set specified by $Pm\bar{3}m$ $1a, b$ leads to the same set of point configurations as $Fm\bar{3}m$ $8c$ or $Ia\bar{3}$ $8a, b$. Each point configuration of this lattice complex can be generated by a properly chosen space group of each of these space-group types.

Configuration-equivalent crystallographic orbits do not necessarily belong to configuration-equivalent types of Wyckoff set.

Example

The orbits of the types of Wyckoff set $Pm\bar{3}m$ $1a, b$ and $Fm\bar{3}$ $8c$ both refer to the set of all conceivable primitive cubic point lattices. Therefore, these two types of Wyckoff set are configuration equivalent and are associated with the same lattice complex. The type of Wyckoff set $P432$ $8g$ x, x, x, however, comprises apart from crystallographic orbits with $x = \frac{1}{4}$ also those with $x \neq \frac{1}{4}$. The orbits with $x = \frac{1}{4}$ refer to the same set of point configurations as $Pm\bar{3}m$ $1a, b$ and $Fm\bar{3}$ $8c$, whereas those with $x \neq \frac{1}{4}$ give rise to point configurations with different properties. As a consequence, the type of Wyckoff set $P432$ $8g$ x, x, x is not configuration equivalent with $Pm\bar{3}m$ $1a, b$ and $Fm\bar{3}$ $8c$, and, therefore, belongs to another lattice complex.

As this example shows, lattice complexes do not form equivalence classes of point configurations, but a certain point configuration may belong to several lattice complexes.

As each type of Wyckoff set uniquely refers to a certain lattice complex, one can also assign all corresponding Wyckoff sets, Wyckoff positions and crystallographic orbits to that lattice complex. A certain lattice complex, however, is frequently related to different types of Wyckoff set.

Among the different types of Wyckoff set belonging to a certain lattice complex, one stands out because its crystallographic orbits show the highest site symmetry. This one is called the *characteristic type of Wyckoff set* of that lattice complex, and the corresponding space-group type its *characteristic space-group type*. All other types of Wyckoff set are referred to as non-characteristic. The term 'characteristic' may also be transferred to particular Wyckoff sets out of the characteristic type. The space groups of all the other types in which the lattice complex may be generated are subgroups of the space groups of its characteristic type.

Different lattice complexes may have the same characteristic space-group type, but then they differ in the oriented site symmetry of their Wyckoff positions within that space-group type.

The characteristic space-group type together with the oriented site symmetry expresses the common symmetry properties of all point configurations of a lattice complex and can be used for its identification. For the purpose of *reference symbols* of lattice complexes, however, instead of the site symmetry the Wyckoff letter of one of the Wyckoff positions with that site symmetry is arbitrarily chosen, as first done by Hermann (1935). This Wyckoff position is called the *characteristic Wyckoff position* of the lattice complex.

Example

$Pm\bar{3}m$ is the characteristic space-group type for the lattice complex of all cubic primitive point lattices. The Wyckoff positions with the highest possible site symmetry $m\bar{3}m$ are $1a$ $0, 0, 0$ and $1b$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$, from which $1a$ has been chosen as the characteristic position. Thus, the reference symbol of this lattice complex is $Pm\bar{3}m$ a.

Example

$Pm\bar{3}m$ is also the characteristic space-group type for a second lattice complex that corresponds to Wyckoff position $8g$ $.3m$ x, x, x. The reference symbol for this lattice complex is $Pm\bar{3}m$ g. Each of its point configurations may be derived by replacing each point of a cubic primitive lattice by eight points arranged at the corners of a cube.

All types of Wyckoff set (together with their Wyckoff sets and Wyckoff positions) that generate, as described above, the same set of point configurations are assigned to the same lattice complex. Accordingly, the following criterion holds: two Wyckoff positions are assigned to the same lattice complex if there is a suitable transformation that maps the point configurations of the two Wyckoff positions onto each other and if their space groups belong to the same crystal family (*cf.* Section 1.3.4.4). Suitable transformations are translations, proper or improper rotations, isotropic or anisotropic expansions or more general affine mappings (without violation of the metric conditions for the corresponding crystal family), and all their products.

By this criterion, the Wyckoff positions of all space groups (1731 entries in the space-group tables, 1128 types of Wyckoff set) are uniquely assigned to 402 lattice complexes. This assignment was first done by Hermann in *Internationale Tabellen zur Bestimmung von Kristallstrukturen* (1935). The corresponding information has also been given by Fischer *et al.* (1973).

The same concept has been used for the point configurations and Wyckoff positions in the plane groups. Here the Wyckoff positions (72 entries in the plane-group tables, 51 types of Wyckoff set) are assigned to 30 plane lattice complexes or net complexes (*cf.* Burzlaff *et al.*, 1968). The complexes for the crystallographic subperiodic groups in three-dimensional space, *i.e.* for the crystallographic point groups, rod groups and layer groups, have been derived by Koch & Fischer (1978*a*).

3.4.1.4. Limiting complexes and comprehensive complexes

As has been shown above, lattice complexes define equivalence classes of orbits but not of point configurations. This property gave rise to the concept of limiting complexes and comprehensive complexes (Fischer & Koch, 1974*a*; Koch, 1974).

For morphological crystal forms an almost analogous situation exists. A certain tetragonal prism, for example, may be a general representative of the crystal form 'tetragonal prism' on the one hand or it may be a special representative of the crystal forms 'tetragonal pyramid' or 'tetragonal disphenoid' on the other hand. In the first case the generating point group may belong to the types $4/mmm$, 422, $4/m$ or $\bar{4}2m$ (with site symmetry 2 for each face), in the second case the types of the generating point group 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 $x \to 0$, 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

references