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14.2. Symbols and properties of lattice complexes

By W. Fischer and E. Koch

14.2.1. Reference symbols and characteristic Wyckoff positions

If a lattice complex can be generated in different space-group types, one of them stands out because its corresponding Wyckoff positions show the highest site symmetry. This is called the *characteristic space-group type* of the lattice complex. The space groups of all the other types in which the lattice complex may be generated are subgroups of the space groups of the characteristic type.

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

The characteristic space-group type and the corresponding oriented site symmetry express the common symmetry properties of all point configurations of a lattice complex. Therefore, they can be used to identify each lattice complex. Within the *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 given, as was first done by Hermann (1935). This Wyckoff position is called the *characteristic Wyckoff position* of the lattice complex.

Examples

(1) $Pm\bar{3}m$ 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 1*a* 000 and 1*b* $\frac{1}{2}\frac{1}{2}\frac{1}{2}$, from which 1*a* has been chosen as the characteristic position. Thus, the lattice complex is designated $Pm\bar{3}m$ *a*.

(2) $Pm\bar{3}m$ is also characteristic for another lattice complex that corresponds to Wyckoff position 8*g* *xxx* $.3m$. Thus, 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.

In Tables 14.2.3.1 and 14.2.3.2, the reference symbols denote the lattice complex of each Wyckoff position. The reference symbols of characteristic Wyckoff positions are marked by asterisks (*e.g.* 2*e* in $P2/c$). If in a particular space group several Wyckoff positions belong to the same Wyckoff set (*cf.* Koch & Fischer, 1975), the reference symbol is given only once (*e.g.* Wyckoff positions 4*l* to 4*o* in $P4/mmm$). To enable this, the usual sequence of Wyckoff positions had to be changed in a few cases (*e.g.* in $P4_2/mcm$). For Wyckoff positions assigned to the same lattice complex but belonging to different Wyckoff sets, the reference symbol is repeated. In $I4/m$, for example, Wyckoff positions 4*c* and 4*d* are both assigned to the lattice complex $P4/mmm$ *a*. They do not belong, however, to the same Wyckoff set because the site-symmetry groups $2/m..$ of 4*c* and $\bar{4}..$ of 4*d* are different.

14.2.2. Additional properties of lattice complexes

14.2.2.1. *The degrees of freedom*

The number of coordinate parameters that can be varied independently within a Wyckoff position is called its number of degrees of freedom. For most lattice complexes, the number of *degrees of freedom* is the same as for any of its Wyckoff positions. The lattice complex with characteristic Wyckoff position $Pm\bar{3}$ 12*j* *m*.. 0*yz*, for instance, has two degrees of freedom. If, however, the variation of a coordinate corresponds to a shift of the point configuration as a whole, one degree of freedom is lost. Therefore, $I4_1$ 8*b* *xyz* is the characteristic Wyckoff position of a lattice complex with only two degrees of freedom, although position 8*b* itself has three degrees of freedom. Another example is given by $P4/m$ 4*j* *m*.. *xy*0 and *P*4 4*d* 1 *xyz*. Both Wyckoff positions belong to lattice complex $P4/m$ *j* with two degrees of freedom.

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 belongs 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 (*P*4 *d*, for example, belongs to the lattice complex with the characteristic position $P4/m$ *j*).

14.2.2.2. *Limiting complexes and comprehensive complexes*

For point groups, the occurrence of limiting crystal forms is well known. In $4/m$, for instance, any tetragonal prism $\{hk0\}$ is a special crystal form with face symmetry *m*.. . In point group 4, on the other hand, the tetragonal prisms $\{hk0\}$ belong, as special cases, to the set of general crystal forms $\{hkl\}$, the tetragonal pyramids, and there is no difference between $\{hkl\}$ and $\{hk0\}$ in either the number or the symmetry of their faces. Therefore, the tetragonal prism is called a 'limiting form' of the tetragonal pyramid. In a case like this, all possible sets of equivalent faces belonging to a special type of crystal form (the tetragonal prism) may also be generated as a subset of another more comprehensive type of crystal form (the tetragonal pyramid). Of course, it is not possible, by considering a tetragonal prism by itself, to decide whether it has been generated by point group $4/m$ or by point group 4. This distinction can be made, however, if the tetragonal prism shows the right striations or occurs in combination with other appropriate crystal forms. Low quartz (oriented point group 321) gives a well known example: the hexagonal prism $\{10\bar{1}0\}$ has the same site symmetry 1 as any trigonal trapezohedron $\{hkil\}$. Therefore, $\{10\bar{1}0\}$ may be recognized as a limiting form only if the crystal shows in addition at least one trigonal trapezohedron.

A similar relation may exist between two lattice complexes. Let *L* be a lattice complex generated by a Wyckoff position of a space group $\mathcal{G}$ (*e.g.* by $P4/mmm$ 4*l* *m*2*m*. *x*00). An appropriate Wyckoff position of a subgroup $\mathcal{H}$ of $\mathcal{G}$ (*e.g.* $P4/m$ 4*j* *m*.. *xy*0) may produce not only all point configurations of *L* but other point configurations in addition (with different orientations of the squares in the example). The complete set then forms a second lattice complex *M*. Such relationships led to the following definition (Fischer & Koch, 1974, 1978):

> If a lattice complex *L* forms a true subset of another lattice complex *M*, the lattice complex *L* is called a *limiting complex* of *M* and the lattice complex *M* a *comprehensive complex* of *L.*

The point configurations of the limiting complex *L* are generated within *M* by restrictions imposed on the coordinate or/and the metrical parameters.

In the above example, such a restriction holds for the *y* coordinate: the condition $y = 0$ for Wyckoff position 4*j* of $P4/m$ filters out exactly those point configurations that constitute the lattice complex $P4/mmm\ l$. The latter complex is, therefore, a limiting complex of the lattice complex $P4/m\ j$. In the present case of restricted coordinates, both complexes belong to the same crystal family and L has fewer degrees of freedom than M.

Another kind of limiting-complex relation is connected with restrictions for metrical parameters. All point configurations of the lattice complex $Pm\bar{3}m\ a$ are also generated by $P4/mmm\ a$ under the restriction $a = c$, *i.e.* in special space groups of type $P4/mmm$. Here L and M have the same number of degrees of freedom, but belong to different crystal families.

Finally, the two types of parameter restrictions for limiting complexes may also occur in combination. The trivariant lattice complex with characteristic Wyckoff position $P4_12_12\ 8b\ xyz$, for example, contains the invariant cubic lattice complex $Fm\bar{3}m\ a$ as a limiting complex. The parameter restrictions necessary are $x = \frac{1}{2}, y = 0, z = \frac{1}{16}, c/a = 4\sqrt{2}$.

As for a limiting form in crystal morphology, it is often impossible to decide by which symmetry (space group and Wyckoff set) a particular point configuration, regarded by itself, has been generated. If a point configuration belongs to a lattice complex that is part of a comprehensive complex, this point configuration is a member of both complexes. As a consequence, the lattice complexes do not form equivalence classes of point configurations. Only if a point configuration is inspected in combination with a sufficient number of other point configurations – like sets of symmetrically equivalent atoms in a crystal structure – does it make sense to assign this point configuration to a particular lattice complex. An example is found in the crystal structures of the spinel type. Here, the oxygen atoms occupy Wyckoff position $32e\ xxx$ in $Fd\bar{3}m$ with $x \approx \frac{3}{8}$ (referred to origin choice 1). If x is restricted to $\frac{3}{8}$, the point configurations generated are those of the lattice complex $Fm\bar{3}m\ a$ (formed by all face-centred cubic point lattices). If for a spinel-type structure this restriction holds exactly, the point configurations of the cations would, nevertheless, reveal the true generating symmetry of the oxygen point configuration. It has, therefore, to be considered a member of the comprehensive complex $Fd\bar{3}m\ e$ rather than a member of the lattice complex $Fm\bar{3}m\ a$ (which includes among others the point configuration of the copper atoms in the crystal structure of copper). For practical applications, a point configuration contained in several lattice complexes may be investigated within the complex that is the least comprehensive but still allows the physical behaviour under discussion. This corresponds to the definition of the symmetry of a crystal generally used in crystallography: the highest symmetry that can be assigned to a crystal as a whole is that of its least symmetrical property known to date.

Even though limiting-complex relations are very useful for establishing crystallochemical relationships between different crystal structures, a complete study has not yet been carried out. Apart from isolated examples in the literature, systematic treatments have been given only for special aspects: plane lattice complexes (Burzlaff *et al.*, 1968); cubic lattice complexes (Koch, 1974); point complexes, rod complexes and layer complexes (Fischer & Koch, 1978); extraordinary orbits for plane groups (Lawrenson & Wondratschek, 1976); noncharacteristic orbits of space groups except those that are due to metrical specialization (Engel *et al.*, 1984). The closely related concepts of limiting complexes and noncharacteristic orbits have been compared by Koch & Fischer (1985).

14.2.2.3. *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, point configurations with the property that the distance between two suitable chosen points is shorter than any small number $\varepsilon > 0$.

Example

Each point configuration of the lattice complex with the characteristic Wyckoff position $P4/mmm\ 4j\ m.2m\ xx0$ 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. Point configurations with $x = 0$ show site symmetry $4/mmm$, their multiplicity is decreased from 4 to 1, and they belong to lattice complex $P4/mmm\ a$.

(ii) The site-symmetry group of any point belonging to the regarded Wyckoff position is not a 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 group of Wyckoff position $Pmma\ 2e\ \frac{1}{4}0z$. As a consequence, the distance between any two symmetrically equivalent points belonging to $Pmma\ e$ cannot become shorter than the minimum of $\frac{1}{2}a, b$ and c.

A lattice complex contains either Wyckoff positions exclusively of the first or exclusively of the second kind. Most lattice complexes are made up from Wyckoff positions of the first kind.

There exist, however, 67 lattice complexes that do not contain point configurations with infinitesimal short distances between symmetry-related points [*cf. Hauptgitter* (Weissenberg, 1925)]. These lattice complexes have been called *Weissenberg complexes* by Fischer *et al.* (1973). The 36 invariant lattice complexes are trivial examples of Weissenberg complexes. In addition, there exist 24 univariant (monoclinic 2, orthorhombic 5, tetragonal 7, hexagonal 5, cubic 5) and 6 bivariant Weissenberg complexes (monoclinic 1, orthorhombic 2, tetragonal 1, hexagonal 2). The only trivariant Weissenberg complex is $P2_12_12_1\ a$. All Weissenberg complexes with degrees of freedom have the following common property: each Weissenberg complex contains at least two invariant limiting complexes belonging to the same crystal family.

Example

$Pmma\ e$ is a comprehensive complex of $Pmmm\ a$ and of $Cmmm\ a$. Within the characteristic Wyckoff position, $\frac{1}{4}00$ refers to $Pmmm\ a$ and $\frac{1}{4}0\frac{1}{4}$ to $Cmmm\ a$.

Except for the seven invariant plane lattice complexes, there exists only one further Weissenberg complex within the plane groups, namely the univariant rectangular complex $p2mg\ c$.

14.2.3. Descriptive symbols

14.2.3.1. *Introduction*

For the study of relations between crystal structures, lattice-complex symbols are desirable that show as many relations between point configurations as possible. To this end, Hermann (1960) derived descriptive lattice-complex symbols that were further developed by Donnay *et al.* (1966) and completed by Fischer *et al.* (1973). These symbols describe the arrangements of the points in the point configurations and refer directly to the coordinate descriptions of the Wyckoff positions. Since a lattice complex, in general, contains Wyckoff positions with different coordinate descriptions, it may be represented by several different descriptive

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references