14.2. Symbols and properties of lattice complexes

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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, $I\bar{4}_1$ 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 $P4$ 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 ($P4$ *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* $m2m.$ *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

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