International Tables for Crystallography (2006). Vol. A, Section 14.2.2.3, p. 849.

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

(*continued on page* 870)

references