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14.1. Introduction and definition

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14.1.1. Introduction

In crystal structures belonging to different structure types and showing different space-group symmetries, the relative locations of symmetrically equivalent atoms nevertheless may be the same (*e.g.* Cl in CsCl and F in CaF_2). The concept of *lattice complexes* can be used to reveal relationships between crystal structures even if they belong to different space-group types.

14.1.2. Definition

The term *lattice complex* (*Gitterkomplex*) had originally been created by P. Niggli (1919), but it was not used by him with an unambiguous meaning. Later on, Hermann (1935) modified and specified the concept of lattice complexes, but the rigorous definition used here was proposed much later by Fischer & Koch (1974) [*cf.* also Koch & Fischer (1978)]. An alternative definition was given by Zimmermann & Burzlaff (1974) at the same time.

To introduce the concept of lattice complexes, relationships between point configurations are regarded.

> The set of all points that are symmetrically equivalent to a given one with respect to a certain space group is called a *point configuration* (*cf.* also crystallographic orbit; Section 8.3.2).

In each space group, there exist infinitely many point configurations. Given a coordinate system, they may be obtained by varying the coordinates x, y, z of a starting point and by calculating all symmetrically equivalent points.

Point configurations refer to the arrangements of atoms in crystal structures. They are analogous to the crystal forms in crystal morphology, where a crystal form is a set of symmetrically equivalent faces. Crystal forms are grouped into types designated by names like 'cube', 'tetragonal dipyramid' *etc*. In a similar, though not strictly analogous way, point configurations are also grouped into types, called lattice complexes. For example, all point configurations forming a cubic primitive point lattice belong to the same lattice complex. Each lattice complex is thus a set of infinitely many point configurations. The following stepwise procedure describes all point configurations belonging to the same lattice complex:

(i) Take all point configurations of a particular Wyckoff position in a particular space group. Mathematically these point configurations are distinguished by the following property: the site-symmetry groups of two arbitrary points from any two of the point configurations are conjugate in the space group (*cf.* Section 8.3.2).

(ii) Collect all point configurations of Wyckoff positions that belong to the same Wyckoff set of a given space group (*cf.* Section 8.3.2). Such Wyckoff positions play an analogous role with respect to this space group. Their point configurations have the following property: the site-symmetry groups of two arbitrary points from any two point configurations are conjugate in the affine normalizer (*cf.* Section 15.3.2) of the space group considered.

(iii) Assemble all point configurations of corresponding Wyckoff sets from all space groups of one of the 219 (affine) space-group types, *i.e.* take all point configurations belonging to a particular type of Wyckoff set (Section 8.3.2). Each affine mapping that maps two space groups of the same type onto each other simultaneously maps onto each other the site-symmetry groups of the points from the point configurations of the corresponding Wyckoff sets.

According to (i), (ii) and (iii), a lattice complex* is defined as follows:

> A *lattice complex* is the set of all point configurations that may be generated within one type of Wyckoff set.

Example

Take, in a particular space group of type $P4/mmm$, the Wyckoff position $4l$ $x00$. The points of each corresponding point configuration form squares that replace the points of the tetragonal primitive lattice referring to Wyckoff position $1a$. For all conceivable point configurations of $4l$, the squares have the same orientation, but their edges have different lengths. Congruent arrangements of squares but shifted by $\frac{1}{2}\mathbf{c}$ or by $\frac{1}{2}(\mathbf{a}+\mathbf{b})$ or by $\frac{1}{2}(\mathbf{a}+\mathbf{b}+\mathbf{c})$ give the point configurations of the Wyckoff positions $4m$, $4n$ and $4o$, respectively, in the same space group. The four Wyckoff positions $4l$ to $4o$, all with site symmetry $m2m.$, make up a Wyckoff set (*cf.* Table 14.2.3.2). They are mapped onto each other, for example, by the translations $\frac{1}{2}\mathbf{c}$, $\frac{1}{2}(\mathbf{a}+\mathbf{b})$ and $\frac{1}{2}(\mathbf{a}+\mathbf{b}+\mathbf{c})$, which belong to the Euclidean (and affine) normalizer of the group. If one space group of type $P4/mmm$ is mapped onto another space group of the same type, the Wyckoff set $4l$ to $4o$ as a whole is transformed to $4l$ to $4o$. The individual Wyckoff positions may be interchanged, however. The set of all point configurations from the Wyckoff positions $4l$ to $4o$ of all space groups of type $P4/mmm$ constitutes a lattice complex. Its point configurations may be derived as described above, but now starting from all space groups $P4/mmm$ with all conceivable lengths and orientations of the basis vectors instead of starting from just a particular group. Accordingly, the point configurations may differ in their orientation, in the size of their squares and in the distances between the centres of their squares.

Just as all crystal forms of a particular type may be found in 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 in each of these space-group types.

All Wyckoff positions, Wyckoff sets and types of Wyckoff set 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

* This definition agrees with that given by Fischer & Koch (1974) and Koch & Fischer (1978), but now the term Wyckoff position is used instead of *Punktlage* or point position, Wyckoff set instead of *Konfigurationslage* or configuration set, type of Wyckoff set instead of *Klasse von Konfigurationslagen* or class of configuration sets. New aspects have been taken into account by Koch & Fischer (1985).

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.* Sections 8.2.7 and 8.2.8). 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.

The same concept has been used for the point configurations and Wyckoff positions in the plane groups. Here the Wyckoff positions (72 entries to the plane-group tables, 51 types of Wyckoff set) are assigned to 30 plane lattice complexes or net complexes (*cf.* Burzlaff *et al.*, 1968).

references