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3.4. Lattice complexes

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3.4.1. The concept of lattice complexes and limiting complexes

3.4.1.1. Introduction

The term *lattice complex* (*Gitterkomplex*) was originally coined by P. Niggli (1919), but he used the term in an ambiguous manner. Later, Hermann (1935) modified and specified the concept of lattice complexes. The rigorous definition used in this chapter was proposed later still by Fischer & Koch (1974*a*) [*cf.* also Koch & Fischer (1978*a*)]. An alternative definition was given by Zimmermann & Burzlaff (1974) at around the same time.

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

The terms 'point configuration' (Fischer & Koch, 1974*a*) and 'crystallographic orbit' (Matsumoto & Wondratschek, 1979) have frequently been used as synonyms for sets of points in three-dimensional space $\mathbb{E}^3$ that are equivalent with respect to a space group $\mathcal{G}$. Such sets of points may be classified in two different ways: (1) according to the concept of lattice complexes (German: *Gitterkomplexe*) and of limiting complexes, which goes back to Hermann (1935) and has been defined more strictly by Fischer & Koch (1974*a*); (2) according to the concept of types of crystallographic orbits and of non-characteristic orbits introduced by Wondratschek (1976). As the two approaches[1] are strongly related but not identical, the classes originating from the two concepts will be compared and the differences worked out.

Both terms, 'point configuration' and 'crystallographic orbit', have been used with two slightly different meanings: (1) for sets of points that are equivalent with respect to a given space group, *i.e.* in the mathematical sense of 'orbit'; (2) for such sets of points, but detached from their generating space groups. The second meaning is referred to, for example, if one speaks only of a primitive cubic point lattice. As within both concepts both meanings are required, one has to distinguish between them. In the following, therefore, the term 'crystallographic orbit' is restricted to the first meaning and the term 'point configuration' is restricted to the second meaning.

3.4.1.2. Crystallographic orbits, Wyckoff positions, Wyckoff sets and types of Wyckoff set

In mathematics, an orbit is a very general group-theoretical term describing any set of objects that are mapped onto each other by the action of a group (*cf.* Section 1.1.7). In fact, orbits are always present in crystallography where equivalence classes are defined by means of a group action (*e.g.* a space-group type is the orbit of a space group in the set of all space groups under the action of the affine group). In the present context, however, the term (crystallographic) orbit will be used in a much more restricted sense, as proposed by Wondratschek (1976):

From any point of $\mathbb{E}^3$, the symmetry operations of a given space group $\mathcal{G}$ generate an infinite set of symmetry-equivalent points, called a *crystallographic orbit with respect to* $\mathcal{G}$ or, for short, a *crystallographic orbit* (*cf.* Section 1.4.4). The space group $\mathcal{G}$ is called the *generating space group* of the orbit.

Each point of a crystallographic orbit defines uniquely a largest finite subgroup of $\mathcal{G}$, which maps that point onto itself, its *site-symmetry group* (*cf.* Section 1.4.4). Site-symmetry groups that belong to different points out of the same crystallographic orbit are conjugate subgroups of $\mathcal{G}$.

Example

The points $x, 0, 0$ and $-x+\frac{1}{2}, 0, \frac{1}{2}$; $-x, 0, 0$ and $x+\frac{1}{2}, 0, \frac{1}{2}$ form an orbit of a given space group *Pmna* together with the infinitely many other points that can be generated from the first four by the translations of *Pmna*. The site-symmetry group 2.. of each such point consists of the identity operation 1 and of a twofold rotation. The position of the twofold axis can easily be read from the corresponding coordinate triplet. The site-symmetry groups of the first two points are $\{1; 2\ x, 0, 0\}$ and $\{1; 2\ x, 0, \frac{1}{2}\}$, respectively. They can be mapped onto another by conjugation *e.g.* with the glide reflection $a\ x, y, \frac{1}{4}$ of *Pmna*. This glide reflection also interchanges the two twofold axes as can easily be learned by inspecting the space-group diagram.

The crystallographic orbits of a given space group $\mathcal{G}$ subdivide the set of all points of $\mathbb{E}^3$ into equivalence classes. It is also possible, however, to define equivalence of orbits on the set of all crystallographic orbits of $\mathcal{G}$:

Two crystallographic orbits of a space group $\mathcal{G}$ belong to the same Wyckoff position (*cf.* Section 1.4.4) if and only if the site-symmetry groups of any two points stemming from the first and the second orbit are conjugate subgroups of $\mathcal{G}$.[2]

Example

The points 0.2, 0, 0 and 0.1, 0, 0.5 belong to different orbits of a given space group *Pmna*. Their site-symmetry groups $\{1; 2\ x, 0, 0\}$ and $\{1; 2\ x, 0, \frac{1}{2}\}$ are conjugate subgroups of *Pmna* (*cf.* the previous example). Therefore, the two orbits belong to the same Wyckoff position of *Pmna*, namely to 4*e*.

The following definition results in a coarser classification of crystallographic orbits:

Two crystallographic orbits of a space group $\mathcal{G}$ belong to the same *Wyckoff set* (German: *Konfigurationslage*, *cf.* Fischer & Koch, 1974*a*) if and only if the site-symmetry groups of any two points stemming from the first and the second orbit are conjugate subgroups of the affine normalizer of $\mathcal{G}$ (*cf.* Section 1.4.4.3).[3]

[1] The following articles are also related to these topics: Engel (1983); Engel *et al.* (1984); Fischer *et al.* (1973); Fischer & Koch (1978, 1983); Koch (1974); Koch & Fischer (1975, 1978*a*, 1985); Steinmann (1984); Wondratschek (1980).

[2] Instead of conjugation by symmetry operations of $\mathcal{G}$, Fischer & Koch (1974*a*) and Koch & Fischer (1975) used inner automorphisms of $\mathcal{G}$.

[3] Instead of conjugation by elements of the affine normalizer of $\mathcal{G}$, Fischer & Koch (1974*a*) and Koch & Fischer (1975) used automorphisms of $\mathcal{G}$.

Accordingly, all orbits of a certain Wyckoff position belong to the same Wyckoff set. The assignment of orbits to Wyckoff sets, therefore, also defines an equivalence relation on the Wyckoff positions of a space group. The Wyckoff sets of the space groups were first tabulated by Koch & Fischer (1975).

Example

In space group *Pmna*, the site-symmetry groups of the points 0.2, 0, 0 and 0.2, 0.5, 0 are {1; 2 x, 0, 0} and {1; 2 $x, \frac{1}{2}$, 0}. There is no symmetry operation from *Pmna* that maps these site-symmetry groups onto another by conjugation and hence the two corresponding orbits do not belong to the same Wyckoff position of *Pmna*. The Euclidian (and affine) normalizer of *Pmna* is a space group of type *Pmmm* with half the lattice parameters compared with those of *Pmna* (*cf.* Chapter 3.5). It contains *e.g.* the twofold rotation 2 $x, \frac{1}{4}, 0$ that maps by conjugation the two site-symmetry groups onto another and also the two axes in the space-group diagram. Therefore, the two orbits belong to the same Wyckoff set even though they belong to the different Wyckoff positions 4*e* and 4*f*.

In analogy to the transition from a single space group to its type, it seems desirable to transfer also the terms 'Wyckoff position' and 'Wyckoff set' to the whole space-group type. For Wyckoff positions, however, such a generalization is not possible: two space groups of the same type can be mapped onto each other by infinitely many isomorphisms or affine mappings. Each isomorphism results in a unique relation between the Wyckoff positions of the two groups, but different isomorphisms may give rise to different relations so that the Wyckoff positions of the same Wyckoff set change their roles.

Such ambiguities, however, cannot occur for Wyckoff sets, because all Wyckoff sets of a certain space group differ in their group-theoretical relations to that group. Therefore, Wyckoff sets may be classified as follows:

Two Wyckoff sets stemming from space groups of the same type belong to the same *type of Wyckoff set* if and only if they are related by an isomorphism (affine mapping) of the two space groups (German: *Klasse von Konfigurationslagen*, *cf.* Fischer & Koch, 1974*a*; Koch & Fischer, 1975). The 219 types of space group in $\mathbb{E}^3$ give rise to 1128 types of Wyckoff set.

Example

Take, in a particular space group of type *P*4/*mmm*, the Wyckoff position 4*l* x, 0, 0. The points of each corresponding orbit form squares that replace the points of the tetragonal primitive point lattice of Wyckoff position 1*a*. For all conceivable orbits of 4*l*, the squares have the same orientation, but their edges differ in their 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 orbits of the Wyckoff positions 4*m*, 4*n* and 4*o*, respectively, in the same space group. The four Wyckoff positions 4*l* to 4*o*, all with site symmetry *m*2*m*., make up a Wyckoff set (*cf.* Table 3.4.3.3). 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 *P*4/*mmm* is mapped onto another space group of the same type, the Wyckoff set 4*l* to 4*o* as a whole is transformed to 4*l* to 4*o*. The individual Wyckoff positions may be interchanged, however, because of the different possible choices for the origin in each individual space group of type *P*4/*mmm*. All the Wyckoff sets 4*l* to 4*o* stemming from all different space groups of type *P*4/*mmm* constitute together a type of Wyckoff set.

3.4.1.3. Point configurations and lattice complexes, reference symbols

For the comparison of crystal structures belonging to different types, another kind of equivalence relationship between crystallographic orbits may be useful:

One may consider the set of points belonging to a certain orbit without paying attention to the generating space group of the orbit. Such a bare set of points is called a *point configuration*. Two crystallographic orbits are called *configuration equivalent* if their point configurations are identical.

This definition uniquely assigns orbits to point configurations, but not *vice versa*.

Example

Let us consider a certain space group of type $Pm\bar{3}m$ with lattice vectors **a**, **b**, **c** together with two of its non-maximal subgroups, namely $Fm\bar{3}$ with index 4 and *P*432 with index 16, both with lattice vectors 2**a**, 2**b**, 2**c**. The orbit of $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ belongs to Wyckoff position 1*b* of $Pm\bar{3}m$ (site symmetry $m\bar{3}m$), and the corresponding set of points, its point configuration, forms a primitive cubic point lattice. As both subgroups have doubled unit-cell edges, the point $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ turns to $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$. The respective orbits belong to Wyckoff position 8*c* of $Fm\bar{3}$ (site symmetry 23.) and to 8*g* of *P*432 (site symmetry .3.), and both correspond to the original point configuration. Therefore, the three orbits $Pm\bar{3}m$ 1*b* $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$, $Fm\bar{3}$ 8*c* $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ and *P*432 8*g* x, x, x with $x = \frac{1}{4}$ are configuration equivalent (together with several other orbits from certain other subgroups of $Pm\bar{3}m$). They all give rise to one and the same point configuration, a specific primitive cubic lattice of points. The generating space group, however, cannot be identified just by looking at the point configuration.

The *eigensymmetry* of a point configuration is the most comprehensive space group that maps this point configuration onto itself. Accordingly, exactly one crystallographic orbit out of each class of configuration-equivalent orbits stands out because its generating space group coincides with the eigensymmetry of its point configuration. In the case of the example above, this specific orbit is $Pm\bar{3}m$ 1*b* (as long as the origin of $Pm\bar{3}m$ remains unchanged).

The concept of configuration equivalence may also be applied to types of Wyckoff set: two types of Wyckoff set are *configuration equivalent* if and only if for each crystallographic orbit belonging to the first type there exists a configuration-equivalent crystallographic orbit belonging to the second type of Wyckoff set, and *vice versa*. All types of Wyckoff set differ in their crystallographic orbits, but configuration-equivalent types of Wyckoff set result in the same set of point configurations.

A *lattice complex* is the set of all point configurations that correspond to the crystallographic orbits of a certain type of Wyckoff set.

There exist 402 classes of configuration-equivalent types of Wyckoff set and, therefore, 402 lattice complexes in $\mathbb{E}^3$.

Example

Let us consider again the type of Wyckoff set *P*4/*mmm* 4*l* to 4*o* (the last example in Section 3.4.1.2). The set of all corresponding point configurations constitutes a lattice complex. Its

references