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 $\mathcal{G}$.