33. On the Crystallographic Space Groupoid

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Some crystal structures are known to have local symmetry elements besides ordinary space-group (global) symmetry elements (Ito, 1950). A complete set of these local symmetry operations and global ones, both operating on one and the same crystal structure, constitute a groupoid defined by Brandt (1926) (Dornberger-Schiff, 1957). However, no clear-cut definition of the crystallographic space groupoid has yet been presented, and accordingly the study to find out the proper position for twinned space groups (Ito, 1935, 1950) in the classes of crystallographic space groupoids has been left intact. In this report we shall deal with these problems.

There exist such partitions of the Euclidean three-space that give rise to polyhedra which are congruent with each other but not related with each other by space-group operations (Hilbert, 1935; Reinhardt, 1928). A point system derived from such a partition is here designated as *hyporegular*. Then, a crystallographic space groupoid must satisfy the condition that the point system derived from it be such a hyporegular point system that can be partitioned into classes of regular point subsystems. Since the structure under consideration is crystallographic, it must conform to a space group to begin with. Therefore, every point in the hyporegular point system must form, with points equivalent to it according to the space-group symmetry, a regular point subsystem. On the other hand, because every crystal structure is built up by dense packing of fundamental regions, it will be a natural extension of this concept that the point system derived from a crystallographic space groupoid is at least hyporegular, its polyhedra forming the fundamental regions for the space groupoid. An example is illustrated in Fig. 1 for a unit cell *ABCD* of such a hyporegular point system as described above. However, because no actual crystal structure according to this symmetry principle has ever been discovered, we denote a space groupoid with this property as *quasi-crystallographic*.

In order to approach significant descriptions of actual crystal structures, we specify the quasi-crystallographic space groupoid by introducing a condition that a congruent embedding exists from a simply connected subspace of a certain regular point system onto a

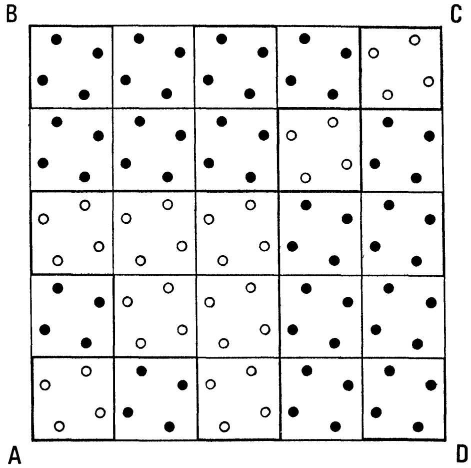

Fig. 1. Unit cell *ABCD* of a hyporegular point system. Distinction of circles, black from white, is only to facilitate easy visualization of the structure; both circles represent points of one and the same hyporegular point system. The tetragonal rotation operation at the centre of each small square is a local symmetry operation.

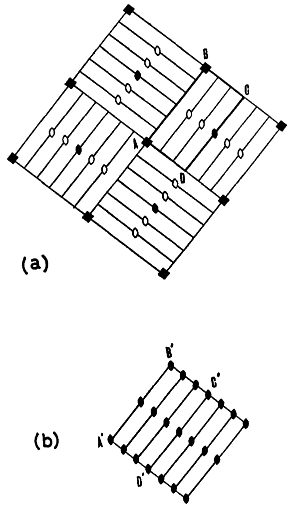

Fig. 2. Crystallographic space groupoid (a). A subspace *A′B′C′D′* of a space group (b) is congruently embedded onto its fundamental region *ABCD*. Open digonal symbols in (a) represent local digonal axes.

fundamental region of the space group contained in a quasi-crystallographic space groupoid. A quasi-crystallographic space groupoid satisfying this condition is called a *crystallographic space groupoid*, an example being given in Fig. 2(a), in which a simply connected subspace $A'B'C'D'$ of space group $P2$ shown in (b) is congruently embedded onto the fundamental region $ABCD$ of space group $P4$. Because the point system derived from a crystallographic space groupoid is hyporegular by definition, the subspace $A'B'C'D'$ of $P2$ must consist of an integral multiple of the fundamental regions of this space group.

Though examples of actual structure cannot be assigned to all the classes of crystallographic space groupoids thus defined, there have been discovered a number of crystal structures that belong to those classes of them for which congruent embeddings are onto fundamental regions of either monoclinic or triclinic space groups. These classes coincide with the *twinned space groups* defined by Ito (1935, 1950).

The special importance of the twinned space groups over the other classes of crystallographic space groupoids rests on the physical nature of crystals; those structures bearing a crystallographic space groupoid are in most cases derived by a transformation from a structure with an ordinary space group, and the mechanism of such a transformation is regularly repeated twinning caused by glidings of atoms along a certain direction in a set of parallel planes in the structure. Since this polysymmetric synthesis postulates an infinite repetition of operation in one direction, the space group compatible with it is either monoclinic or triclinic.

References

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