47. On the Local Condition of the Regular Point System

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The regular point system (RPS), the basis upon which the entire edifice of the theory of space groups is built, is defined as a discrete and homogeneous distribution of points which possesses the same arrangement of points around each point (Hilbert and Cohn-Vossen, 1932, p. 50). This condition of the RPS can be interpreted as follows: The sets, ε_∞ 's, of an infinite number of vectors from each point to all the other points of the system are equal to one another; arbitrarily chosen two such sets are either congruent or reflection-symmetric with each other.

With this feature of the RPS in mind, we can sketch out its important property as follows: Take the shortest vector P_0P_1 from a given point P_0 of our system and construct a plane perpendicular to P_0P_1 at its midpoint. Apply the same procedure to the second shortest vector in the set ε_∞ from P_0 , to the third shortest, and so on. Then, we shall eventually arrive at a Dirichlet polyhedron made up of these planes and containing only one point, P_0 , of the RPS as illustrated in Fig. 1. The entire space of the RPS is completely filled with equal Dirichlet polyhedra, two adjacent ones holding a face in common. Those points which provide the Dirichlet polyhedron around P_0 with faces are defined as the points 'nearest' to P_0 and

Fig. 1. Construction of the Dirichlet polygon $ABCDE$ around P_0 . A part of an RPS with the symmetry of $p4$ is shown. $P_1, P_2, \dots$ and P_5 are the points 'nearest' to P_0 , no other points contributing to the generation of the polygon.

the set of vectors from P_0 to these nearest points is denoted by ε_k (Vainshtein, 1981, p. 149). Then, the equality of Dirichlet polyhedra in the RPS is equivalent to the equality of ε_k 's.

Take a point A in an infinite, discrete and homogeneous point system and construct a sphere S with centre A and radius r . Denote by P_A a set of vectors from A to all the points on and within the sphere S . If r is appropriately chosen, the local condition holds: If P_A 's are equal for every point, the system is regular (Delone *et al.*, 1976). In Vainshtein's text book on crystallography recently published, mention is made of this local condition (Vainshtein, 1981, p. 148), where the author has attempted a translation of the topological language of spherical neighbourhoods in the original paper into the geometrical language of Dirichlet polyhedra. This geometrical interpretation is supposed to be significant in view of its possible relation to the physical causes for the formation of the crystalline structure. However, in order to express P_A in terms of ε_k , we must supply an answer to the question whether the equality of ε_k 's can be a condition sufficient for the point system to be regular; whether the equality of Dirichlet polyhedra can ensure a unique way of their joining. While the answer to this question is affirmative for asymmetric polyhedra with asymmetric faces (Vainshtein, 1981, p. 150), it has been mentioned that two-dimensional point systems can be irregular even if the equality of ε_k 's holds (Delone *et al.*, 1976, p. 20, Comment). We shall demonstrate below a three-dimensional example for which the answer is negative.

Let us begin with a two-dimensional case. In Fig. 2, we construct a convex pentagon $ABCDE$ around a point P_0 under the conditions: $P_0A = P_0B = P_0E$, $AB \neq AE$, $BC \parallel ED$ and these two lines are equally separated from P_0 , and $CD \perp BC$. If we try to joint such

Fig. 2. Pentagon to be the Dirichlet polygon in the point system in Fig. 4. $P_0A = P_0B = P_0E$, $AB \neq AE$, $BC \parallel ED$ and these two lines are equally separated from P_0 , and $CD \perp BC$.

Fig. 3

Fig. 4

Figs. 3-4. 3: Two ways, A and B, of joining pentagons. Each of the figures shows a part of a horizontal band infinitely extended. 4: Two-dimensional structure disordered by randomly mixing the two kinds of band, A and B, in Fig. 3.

pentagons together to cover a plane with them, we shall immediately find that two alternative ways of their joining are possible as shown in Fig. 3, A and B. If we randomly mix these two ways of joining in our process of covering the plane, we shall arrive at a disordered two-dimensional structure as illustrated in Fig. 4, where we can easily recognize that our pentagons play the role of Dirichlet polygons in the point system consisting of their P_0 's. Therefore, while the equality of ε_k 's holds, this point system is not regular because it is disordered.

In Fig. 5A is given a polyhedron around P_0 whose front and back faces are parallel to each other and equal to the pentagon in Fig. 2 and whose basal face is square and perpendicular to the above faces. It will not be difficult to see, with reference to the previous two-dimensional case, that the polyhedra equal to the one in Fig. 5A can fill the space completely and they will then turn out to be the Dirichlet polyhedra in the point system of their P_0 's. When two such polyhedra are joined together with the basal face in common, one of them can take four distinct orientations with respect to the other according to the rotations of the former by $\pi/2$ and its multiples about a vertical axis passing P_0 's as shown in Fig. 5, B and C. This means that upon joining these polyhedra together, four distinct

Fig. 5. Dirichlet polyhedron capable of causing disordered structures. A: The polyhedron is reflection-symmetric across the plane indicated by dashed lines. The section along this plane, on which P_0 lies, is equal to the pentagon in Fig. 2. B and C: When two polyhedra are joined together along the square basal face, one of them can be rotated with respect to the other about a vertical axis by $\pi/2$ and its multiples.

ways of layer stacking are possible, which leads to the same argument as in the previous two-dimensional case. It has thus been concluded that the equality of Dirichlet polyhedra does not necessarily determine the way of their joining.

P_A defined by Delone *et al.* contains not only ε_k but also vectors to 'next nearest' points so that P_A can always determine the way of joining Dirichlet polyhedra. In fact, if we take a set of vectors ε_n from P_0 to its nearest and next nearest points, both the equality of ε_k 's and a unique way of their joining will ensue from the equality of ε_n 's.

References

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