Symmetry of STRUCTURE

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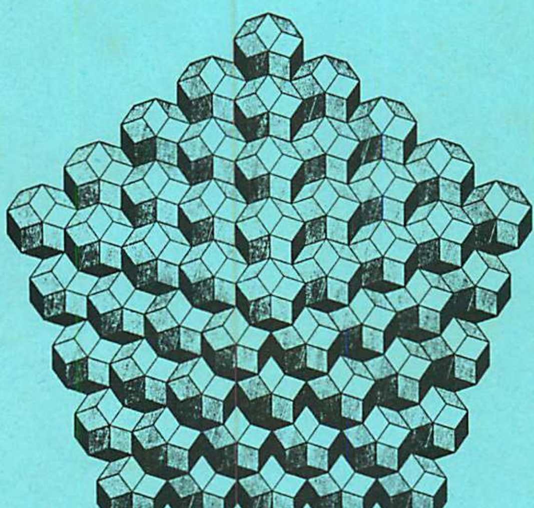
Abstracts

I.



Edited by Gy. Darvas and D. Nagy

Buda
pest

August 13-19, 1989

hungary

ON 3-PERIODIC MINIMAL SURFACES. I. SYMMETRY AND DERIVATION.

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A **minimal surface** in 3-dimensional space R^3 is defined as a surface with mean curvature zero at each of its points, i.e. the two extreme values of curvature (main curvatures) are equal in magnitude but opposite in sign for each point of the surface. Thus all points of a minimal surface are saddle points.

In crystallography, especially those minimal surfaces have attracted attention that are periodic in three independent directions and, therefore, may be related to crystal structures. In this connection mainly those surfaces that are free of self-intersections seem to be of interest. Such a surface subdivides R^3 into two regions or labyrinths such that each labyrinth is connected but not simply connected. If the two labyrinths are congruent the intersection-free, 3-periodic minimal surface is called a **minimal balance surface** (Fischer & Koch, 1987).

The symmetry of a minimal balance surface is best characterized by a pair of space groups G-H: G describes the full symmetry of the (non-oriented) surface, and H is that subgroup of G with index 2 which consists of all symmetry operations that do not interchange the two sides of the surface and the two labyrinths. Obviously, the pairs G-H correspond uniquely to the proper black-white space groups (cf. also Mackay & Klinowski, 1986).

Let us consider a symmetry operation s of G that does not belong to H. Then s interchanges the two sides of each minimal balance surface with symmetry G-H, and all fixed points of s must lie on the surface. This property, however, is inconsistent with the absence of self-intersections for minimal balance surfaces if s is a 3-, 4- or 6-fold rotation, a reflection or a 6-fold rotoinversion. As a consequence, certain space-group pairs G-H are incompatible with minimal balance surfaces. A detailed examination of the 1156 types of group-subgroup pairs with index 2 shows that - for the reasons described above - only 547 of them are not incompatible with minimal balance surfaces.

For these 547 types of space-group pairs all 2-fold rotation axes and all (roto)inversion centres $\bar{1}$, $\bar{3}$ and $\bar{4}$ have been tabulated that must be located on each minimal balance surface with that symmetry (Koch & Fischer, 1988). This knowledge gives an aid for the derivation of new families of minimal balance surfaces. Especially useful are 2-fold rotation axes which exist for 352 out of the 547 types. Considering only the sets of all 2-fold axes belonging to G but not to H, 52 different configurations of straight lines on minimal balance surfaces result. In 18 of these cases all 2-fold axes are 3-dimensionally connected, in 12 cases they form infinite sets of parallel plane nets. Both situations are favourable for the derivation of minimal balance surfaces:

(1) In a 3-dimensional connected set of 2-fold axes skew polygons are formed that may be spanned by **disk-like surface patches.** Such a surface patch may be continued with the aid of those 2-fold rotations that correspond to its straight edges. If the original skew polygon has been adequately chosen the resulting infinite surface is free of self-intersections, i.e. it is a minimal balance surface. An adequately chosen skew polygon has to fulfill the following conditions: (i) All its vertex angles must be chosen as small as possible; in particular, no angles larger than 90° are allowed. (ii) The skew polygon must not be penetrated by a further 2-fold axis belonging to the same set.

The 18 configurations of 3-dimensionally connected 2-fold axes give rise to 15 families of minimal balance surfaces that may be generated from disk-like spanned skew polygons (cf. Schoen, 1970; Fischer & Koch, 1987; Koch & Fischer, 1988). Eight of these families had not been known before.

(2) The 12 configurations of 2-fold axes that disintegrate into parallel plane nets are compatible with different kinds of surface patches. Again an original surface patch may be continued with the aid of the 2-fold rotations referring to its boundaries.

(i) If all plane nets are congruent and if at least half the polygon centres for a pair of adjacent nets lie directly above each other, **catenoid-like surface patches** may be spanned between neighbouring polygons from adjacent nets. Such catenoids give rise to seven families of minimal balance surfaces (cf. Schoen, 1970; Koch & Fischer, 1988), one of which had not been described before.

(ii) If plane nets of two different kinds are stacked alternately upon each other surface patches may be spanned that have been called **branched catenoids.** A branched catenoid is bounded by a convex polygon at one end and by a concave polygon with one point of self-contact at its other end. The convex polygon stems from one of the more wide-meshed nets, whereas the concave polygon is formed by two, three or four polygons with a common vertex of an adjacent close-meshed net. Branched catenoids refer to three new families of minimal balance surfaces (Fischer & Koch, 1989a).

(iii) Congruent parallel plane nets stacked directly upon each other allow surface patches that have been called **multiple catenoids.** A multiple catenoid may be imagined as resulting from fusion of two, three, four or six neighbouring catenoids. It is bounded by two congruent concave polygons with one point of self-contact each. Multiple catenoids give rise to eight new families of minimal balance surfaces (cf. Karcher, 1988; Koch & Fischer, 1989a).

(iv) Configurations of 2-fold axes that disintegrate into parallel plane quadrangular nets are compatible with 1-dimensionally infinite surface patches, called **infinite strips.** Such an infinite strip is bounded by two infinite (zigzag or meander) lines. The strips may be regarded as resulting from fusion of an infinite row of neighbouring catenoids. In most cases infinite strips constructed in this way produce minimal surfaces that may be also built up from finite surface patches as described above. In two cases, however, minimal surfaces of new families are formed (Fischer & Koch, 1989b).

(v) For configurations of 2-fold axes that disintegrate into congruent plane parallel nets stacked directly upon each other the catenoid-like surface patches [cf. (i)] may be replaced by more complicated ones, called **catenoids with spout-like attachments**. For this, spouts are attached to the "faces" of the catenoids resulting in surface patches with two, three or four additional ends that are not bounded by straight lines. Spouts of neighbouring catenoids are united to handles or to three-armed or four-armed handles, respectively. Six families of minimal balance surfaces correspond to such surface patches (Koch & Fischer, 1989b); only one of these families had been described before (Schoen, 1970).

In addition, two families of minimal balance surfaces have been derived which contain skew 2-fold axes in three independent directions (Fischer & Koch, 1987, 1989c; Koch & Fischer, 1988).

Two families of minimal balance surfaces without 2-fold axes are known so far, the gyroid surfaces (cf. Schoen, 1970; Fischer & Koch, 1987) and orthorhombically distorted P surfaces (cf. Karcher, 1988; Fischer & Koch, 1989c).

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