SHORT COMMUNICATIONS

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Triply periodic minimal balance surfaces: a correction.

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Abstract

In previous papers, 15 families of minimal balance surfaces that can be generated with the aid of disc-like surface patches were noted. Recently, it has become apparent that the inherent symmetry of two of these families, the $C(S)$ surfaces and the Y surfaces, is higher than the symmetry used for their generation. As a consequence, $C(S)$ surfaces are in fact P surfaces and Y surfaces are in fact D surfaces.

Triply periodic minimal surfaces are complicated infinite geometrical objects that cannot easily be characterized. Therefore, finite surface patches are often used for their description. To that end, an infinite minimal surface must be subdivided into infinitely many congruent finite surface patches, all of which are symmetrically equivalent. The boundaries of such surface patches should not be too complicated. The entire infinite surface may be generated from one of these surface patches by systematic continuation with the aid of symmetry. The point group of the original surface patch together with all those symmetry operations that allow the continuation of this surface patch beyond its boundaries form a set of generators of a space group, called the generating symmetry of the surface (Fischer & Koch, 1987). Two different minimal surfaces belong to the same family if they have been produced by continuation of analogous surface patches with the aid of analogous symmetry operations. On the other hand, certain less-complicated triply periodic minimal surfaces may be formed with the aid of various generating symmetries and starting from several dissimilar simple surface patches. In that case, the generating symmetry of a minimal surface may differ from its inherent symmetry, *i.e.* the group of all symmetry operations that map the surface onto itself. Then the generating symmetry is a true subgroup of the respective inherent symmetry.

A well known example illustrating such a situation is based on Schwarz's P surface (Schwarz, 1890). Each surface of this family may be generated either from a disc-like surface patch spanning a skew quadrangle (generating symmetry $Im\bar{3}m$-$Pm\bar{3}m$) or from another disc-like surface patch spanning a skew hexagon ($Fd\bar{3}m$-$F\bar{4}3m$; see Schoenflies, 1891; Andersson, Hyde & von Schnering, 1984; Fischer & Koch, 1987; Koch & Fischer, 1992).

The comparison of two minimal surfaces is facilitated by examining their genera. The genus of a triply periodic surface must be associated with a finite part of that surface since otherwise its value would become infinite. For triply periodic minimal surfaces, the genus is associated with a primitive unit cell of the space group that describes its inherent symmetry. For a minimal balance surface, *i.e.* a triply periodic intersection-free minimal surface subdividing R^3 into two congruent regions, its inherent symmetry may be best described by a group-subgroup pair G_i-H_i of space groups with index 2. Then the genus must be associated with a primitive unit cell of the subgroup H_i (Fischer & Koch, 1989).

The genera of two distinct triply periodic minimal surfaces from the same family are necessarily equal and the equality of the genera is a necessary condition for two triply periodic minimal surfaces generated from dissimilar surface patches to belong to the same family. Among others, this criterion has been used in earlier papers to decide whether or not a newly derived minimal balance surface belongs to a new family or to a family that is already known.

If, however, the genus of a minimal (balance) surface is calculated erroneously from some generating symmetry $(G_g$-$)H_g$ that differs from the inherent symmetry $(G_i$-$)H_i$ then the calculated value of the genus may be too high. This occurs whenever H_g is not a translation-equivalent subgroup of H_i because then the primitive unit cell of H_g is larger than that of H_i.

Such a mistake was made with regard to two families of minimal balance surfaces designated $C(S)$ and Y (Fischer & Koch, 1987). They have been derived from disc-like surface patches, namely skew octagons and skew hexagons, respectively. The corresponding generating symmetry is $Ia\bar{3}d$-$Ia\bar{3}$ for the $C(S)$ surfaces and $I4_132$-$P4_332$ for the

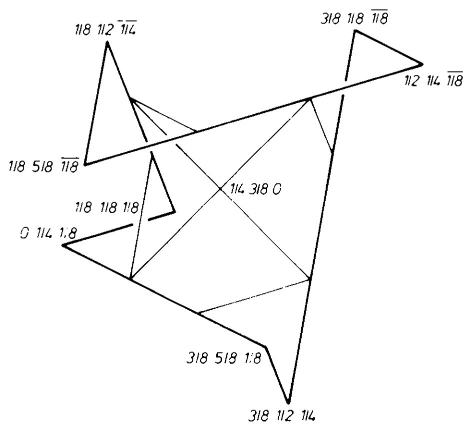

Fig. 1. Skew octagon with site symmetry $\bar{4}$..-2.. subdivided into eight congruent skew quadrangles forming generating polygons of a P surface. The coordinates of the centre and the vertices of the octagon refer to a conventional description of $Ia\bar{3}d$.

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Y surfaces. It had not been realized that in both cases the inherent symmetry of the surfaces is higher, namely $Im\bar{3}m$–$Pm\bar{3}m$ and $Pn\bar{3}m$–$Fd\bar{3}m$, respectively. As a consequence, $C(S)$ surfaces are in fact P surfaces and Y surfaces are in fact D surfaces (*cf.* Koch & Fischer, 1992).

Fig. 1 shows a skew octagon with site symmetry $\bar{4}$..-2.. as was used for the generation of $C(S)$ surfaces. The octagon is subdivided by straight lines into eight congruent skew quadrangles and each of these quadrangles represents a generating polygon of a P surface as described, for example, in Table 2 of Fischer & Koch (1987). In fact, inspection of a model of the $C(S)$ surface shows the additional straight lines that form the boundaries of the small quadrangles.

Fig. 2 displays a skew hexagon with site symmetry ..2-..2 as was applied to derive the Y surfaces. The indicated subdivision yields eight congruent skew quadrangles, each of which can be used to generate a D surface (*cf.* Table 2 of Fischer & Koch, 1987).

The genus of the $C(S)$ and Y surfaces was stated to be 9 in previous papers (see, for example, Koch & Fischer, 1988; Fischer & Koch, 1989), whereas P surfaces as well as D surfaces have genus 3. The difference of these values is caused by the different sizes of the primitive unit cells of H_i and H_g. As the following diagrams show, the primitive unit cell of H_g is four times the size of H_i in both cases.

P surface:

$$\begin{array}{ccc} Im\bar{3}m(a) & - & Pm\bar{3}m(a) \\ \mid 2 & & \mid 2 \\ Pm\bar{3}n(a) & - & Pm\bar{3}(a) \\ \mid 4 & & \mid 4 \\ Ia\bar{3}d(2a) & - & Ia\bar{3}(2a) \end{array}$$

D surface:

$$\begin{array}{ccc} Pn\bar{3}m(a) & - & Fd\bar{3}m(2a) \\ \mid 2 & & \mid 2 \\ P4_232(a) & - & F4_132(2a) \\ \mid 4 & & \mid 4 \\ I4_132(2a) & - & P4_332(2a) \end{array}$$

An enlargement of the unit cell by a factor of n results in a change of the genus g to

$$g_n = 1 + n(g-1)$$

as shown earlier (Fischer & Koch, 1989). The values $n = 4$ and $g = 3$ (the genus of P and D surfaces) yield $g_n = 9$, the incorrectly stated genus of $C(S)$ and Y surfaces.

For all minimal balance surfaces known so far it has been checked that a similar error does not occur.

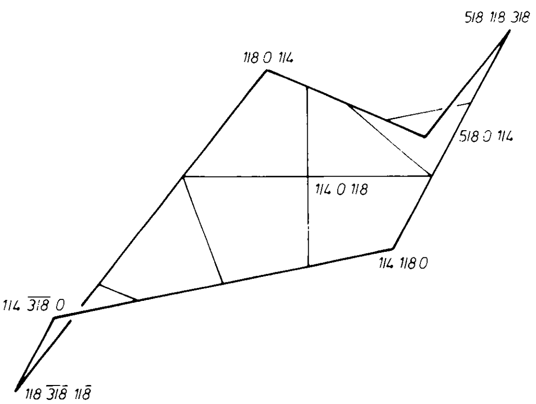

Fig. 2. Skew hexagon with site symmetry ..2-..2 subdivided into eight congruent skew quadrangles forming generating polygons of a D surface. The coordinates of the centre and the vertices of the hexagon refer to a conventional description of $I4_132$.

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Kitajgorodskij's categories.

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Abstract

To a close approximation, the relative frequency of the space groups of molecular organic compounds is determined by ease of packing. Kitajgorodskij, with molecular organic structures in mind, divided the space groups of the triclinic, monoclinic and orthorhombic systems into four categories: 'closest-packed', 'limitingly close-packed', 'permissible' and 'impossible' [Китайгородский (1955). Органическая Кристаллохимия. Москва: Изд. Акад. Наук; Engl. transl: Kitaigorodskii (1961). *Organic Chemical Crystallography*. New York: Consultants Bureau]. Empirically, about a dozen of the 'impossible' space groups are not rare and several of them (Pc, $P2/c$, $C222_1$, $Fdd2$ and possibly other orthorhombic groups) can be recategorized as 'permissible' on Kitajgorodskij's own criteria. In addition, certain space groups (notably $C2/c$ and $Pbca$) requiring inherent molecular symmetry for close packing in

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