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To cite this version:
Veit Elser. Space filling minimal surfaces and sphere packings. Journal de Physique I, EDP Sciences, 1994, 4 (5), pp.731-735. <10.1051/jp1:1994172>. <jpa-00246943>

HAL Id: jpa-00246943
https://hal.archives-ouvertes.fr/jpa-00246943
Submitted on 1 Jan 1994

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Space filling minimal surfaces and sphere packings

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(Received 25 October 1993, accepted in final form 20 January 1994)

Abstract. — A space filling minimal surface is defined to be any embedded minimal surface without boundary with the property that the area and genus enclosed by any large spherical region scales in proportion to the volume of the region. The triply periodic minimal surfaces are one realization, but not necessarily the only one. By using the genus per unit volume of the surface, a meaningful comparison of surface areas can be made even in cases where there is no unit cell. Of the known periodic minimal surfaces this measure of the surface area is smallest for Schoen's F-RD surface. This surface is one of several that is closely related to packings of spheres. Its low area is largely due to the fact that the corresponding sphere packing (fcc) has the maximal kissing number.

The triply periodic minimal surfaces have found expression in a diverse variety of physical structures [1]. The basic length scale of these structures is set by the dimensions of their primitive unit cells. On much larger length scales they appear as a foam which fills space homogeneously. Considered as an example of a thermodynamic phase in equilibrium, the macroscopic homogenity of a foam is more significant than its microscopic periodicity. This fact is nicely illustrated by the existence of quasicrystals in metallurgy. Are there analogous quasicrystalline minimal surface foams? In anticipation that the answer to this question is «yes», I consider below the use of topology — as opposed to periodicity — in normalizing measurements of a surface. Of the known triply periodic minimal surfaces, the one with the smallest value of the topologically normalized surface area is Schoen's F-RD surface [2]. In trying to understand this fact I am lead to consider a family of minimal surfaces closely related to sphere packings. The surface areas of such surfaces are reproduced to a remarkable degree of accuracy by a formula involving the packing fraction \( f \), kissing number \( k \), and kissing angle \( \theta \) of the corresponding sphere packing.

Essentially the same scale invariant quantity defined below was introduced by Anderson et al. [3] and by Hyde [4] in his definition of the « packing index » of a minimal surface. In addition to its geometrical significance, considered here, this index is believed to be correlated
with the phase stability of a sequence of cubic phases in the DDAB-water-styrene system [5], and measurable, in principle, by NMR techniques [6].

Consider an embedded minimal surface without boundary and any sequence of spherical volumes $V(R)$ with increasing radius $R$. Let $A(R)$ be the area and $G(R)$ the genus of the surface inside $V(R)$. The surface will be called «space filling» if the following two limits exist:

1. \[
  a_{\text{vol}} = \lim_{R \to \infty} \frac{A(R)}{V(R)},
\]
2. \[
  g_{\text{vol}} = \lim_{R \to \infty} \frac{G(R)}{V(R)}.
\]

The limits $a_{\text{vol}}$ and $g_{\text{vol}}$ are respectively the area and genus «per unit volume». Confusion about the value of $g_{\text{vol}}$ for periodic surfaces can be avoided by using the asymptotic relation [7]

\[
  G(R) \sim -\frac{\chi(R)}{2} + O(R^2),
\]

where $\chi(R)$ is the Euler characteristic of the surface inside $V(R)$ (1). The Euler characteristic has the advantage over the genus in being additive for two surfaces being joined along a closed curve (such as considered below). In a crystalline surface the situation is simplest when the unit cell cuts the surface so that each boundary curve lies entirely within one of the cell's faces. The Euler characteristic of the crystal is then just $\chi_{\text{cell}}$, the Euler characteristic inside one primitive cell, times the number of unit cells. Using (3) one may define the genus «per primitive cell» as well as the genus «per unit volume»:

\[
  g_{\text{cell}} = -\frac{\chi_{\text{cell}}}{2} = g_{\text{vol}} \nu_{\text{cell}},
\]

where $\nu_{\text{cell}}$ is the volume inside one primitive cell. With this definition $g_{\text{cell}}$ is one less the «genus» conventionally associated with the compactified surface [7] (e.g. $g_{\text{cell}} = 2$ for the P surface). A dimensionless combination of $a_{\text{vol}}$ and $g_{\text{vol}}$ (and proportional to $a_{\text{vol}}$) defines the topologically normalized surface area of a space filling minimal surface:

\[
  a = \frac{a_{\text{vol}}}{g_{\text{vol}}^{1/3}}.
\]

Table I.

<table>
<thead>
<tr>
<th>Surface</th>
<th>Sphere packing</th>
<th>$k$</th>
<th>$f$</th>
<th>$\theta$</th>
<th>$r$</th>
<th>$a(k, f, \theta)$</th>
<th>$a$</th>
</tr>
</thead>
<tbody>
<tr>
<td>D</td>
<td>diamond</td>
<td>4</td>
<td>0.340</td>
<td>54.7°</td>
<td>1.016</td>
<td>1.898</td>
<td>1.919</td>
</tr>
<tr>
<td>P</td>
<td>sc</td>
<td>6</td>
<td>0.524</td>
<td>45°</td>
<td>1.148</td>
<td>1.859</td>
<td>1.861</td>
</tr>
<tr>
<td>I-WP</td>
<td>bcc</td>
<td>8</td>
<td>0.680</td>
<td>35.3°</td>
<td>1.199</td>
<td>1.923</td>
<td>1.908</td>
</tr>
<tr>
<td>F-RD</td>
<td>fcc</td>
<td>12</td>
<td>0.740</td>
<td>30°</td>
<td>1.195</td>
<td>1.770</td>
<td>1.758</td>
</tr>
</tbody>
</table>

(1) Equation (3) is also valid for nonperiodic surfaces provided the error term, proportional to the number of boundary curves generated at the surface of $V(R)$, remains subdominant.
The « packing index » of a minimal surface, as defined by Hyde [4], is just $\sqrt{a^2/2}$; the index defined by Anderson et al. [3] is $a^3/\pi$. Values of $a$ for four periodic minimal surfaces are given in the last column of table I. The small dispersion in these numbers is remarkable. Obtaining bounds on $a$ appears to be a difficult problem. Of the known periodic surfaces for which surface areas are known, the F-RD surface has the minimum value of $a$ [3, 4].

The F-RD surface and the three others in table I each belong to a one parameter family of constant mean curvature surfaces which terminates in a packing of identical spheres [7]. This greatly facilitates the visualization of these surfaces since one may begin with the corresponding sphere packing and then replace the regions around the contact points by catenoids as shown in figure 1. The limit of the F-RD family of constant mean curvature surfaces is the fcc packing of spheres — the lattice packing which achieves both the maximum packing fraction ($f = 0.740$) and kissing number ($k = 12$). An approximate calculation below shows that it is the latter which is responsible for giving the F-RD surface the smallest value of $a$.

Consider a general packing of identical spheres where each sphere has radius $r > 1$ and makes contact with exactly $k$ other spheres. Figure 1 shows one sphere centered at $A$ making contact with two other spheres; the separation between « kissing » spheres is $AB = 2r$. The arrangement of kissing spheres may vary from sphere to sphere; even so, there is a minimum angle $2\theta$ subtended by any pair of kissing spheres. For the particular packing considered in figure 1 we will assume this minimum angular separation is realized by the two spheres making contact with sphere $A$. Smaller spheres, concentric with the original spheres of the packing, can be joined together smoothly by catenoids. The transformation of each small sphere (see Fig. 1) corresponds to the replacement of $k$ spherical caps by $k$ half-catenoids which smoothly join the surface of the small sphere. At each circular junction between sphere and catenoid, the first derivatives are continuous. This cannot be extended to the second derivatives since the two surfaces clearly have different constant values of mean curvature. In order to have the largest possible fraction of catenoid (zero mean curvature) surface, the small spheres are made as small as possible without, of course, allowing catenoids to intersect each
other. The optimal construction is shown in figure 1 where two catenoids at the minimum angular separation just touch each other at C. By rescaling the small sphere radius \( \overline{AC} \) to 1, the radius of spheres in the packing is given by

\[
 r = \cos \theta + (\sin \theta)^2 \text{arcsinh} (\cot \theta).
\]

(6)

The areas of one eliminated spherical cap and one replacement half-catenoid are given respectively by

\[
a_{\text{cap}} = 2\pi (1 - \cos \theta),
\]

(7)

\[
a_{\text{cat}} = \pi r \sin^2 \theta.
\]

(8)

Viewing each of the small punctured spheres with its \( k \) half-catenoids as a node of an approximate minimal surface, we obtain for the area per node the expression

\[
a_{\text{node}} = 4\pi + k(a_{\text{cat}} - a_{\text{cap}}).
\]

(9)

The area per unit volume of the approximate minimal surface is obtained by dividing the area per node by the volume associated with each node, \( \nu_{\text{node}} \). Since the latter is just the volume per sphere of the sphere packing, it is simply related to the packing fraction by

\[
f = \left( \frac{4}{3} \pi r^3 \right) / \nu_{\text{node}}.
\]

(10)

Similarly, the genus per unit volume is obtained by dividing the genus per node, \( g_{\text{node}} \), by \( \nu_{\text{node}} \). Again using (3), but this time applied to a node rather than a primitive cell, we have \( g_{\text{node}} = -X_{\text{node}}/2 \) since the entire surface is constructed by joining together a large number of nodes, always along circular boundary curves. Finally, since the Euler characteristic of a sphere with \( k \) holes is \( 2 - k \), we obtain

\[
g_{\text{node}} = \frac{k}{2} - 1.
\]

(11)

Dividing (9) and (11) by \( \nu_{\text{node}} \) to form \( a_{\text{vol}} \) and \( g_{\text{vol}} \) and using these in (5), we arrive at the topologically normalized surface area of our approximate minimal surface:

\[
a(k, f, \theta) = \left( \frac{9 \pi f^2}{k - 2} \right)^{1/3} \left( \frac{2 - k(1 - \cos \theta)}{r^2} + \frac{k \sin^2 \theta}{2r} \right).
\]

(12)

We note that the \( r \) in (12) is not an independent parameter but given explicitly by (6). Formula (12) is compared with the surface areas of the true minimal surfaces in table I. The agreement is quite good considering the fact that pieces of the original spheres — having positive Gaussian curvature — remain in the approximate minimal surface. To the extent that the mean curvature of the approximate surface is not constant, its surface area should be greater than that of a constant mean curvature surface enclosing the same volume. However, the enclosed volume of the approximate surface does not correspond exactly to that of the true zero mean curvature surface. This leads to an underestimate of the surface area since all four surfaces considered here have maximum area at the true volume fraction [7]. The two sources of error (non-constant mean curvature, wrong volume) have opposite signs and may partially compensate each other. Nevertheless, the correct identification of the smallest area minimal surface (F-RD) is probably not fortuitous and formula (12) gives some explanation of this outcome. We see immediately that it is not the packing fraction but the rather large kissing number that is responsible for the small area.
A definite shortcoming of the sphere packing representation of minimal surfaces is the asymmetrical treatment of the inside and outside volumes. Surfaces which possess this symmetry, such as P and D, actually lead to two different approximations, depending on what one considers to be the « inside » and « outside ». This discrepancy can be illustrated for the case of the P surface by computing the location of the « flat points » — which in fact are not flat at all in the approximation and are better defined as the points of intersection with axes of 3-fold symmetry. In a \( 1 \times 1 \times 1 \) unit cell the flat point coordinates are given by \( (\pm x, \pm x, \pm x) \) where \( x = 1/4 \) in the exact surface. In the approximate surface, with the choice made of putting the spheres at the integer coordinates, we find instead \( x = 1/(2 \sqrt{3} r) = 0.2515 \). Additional shortcomings of the approximation considered here can be expected in the case of surfaces, such as C(P) [7], where the corresponding family of constant mean curvature surfaces terminates in self-intersecting spheres.

The close correspondence between the F-RD minimal surface and the fcc sphere packing suggests some possibilities for other minimal surfaces, in particular, surfaces which are not periodic. Viewing the fcc packing as a particular periodic sequence (...)ABCABC...) of close-packed planes of spheres, I speculate that other sequences — quasiperiodic, random — also correspond to minimal surfaces. The parameters \( k, f, \) and \( \theta \) would be the same in each case so that their topologically normalized areas would all be close to that of the F-RD surface. In this regard there are two interesting problems: (1) Among these possibilities, does the F-RD surface remain the surface with the smallest topologically normalized area? (2) Can the corrections to formula (12) for this class of surfaces be understood directly in terms of the layering sequence?

Acknowledgments.

This work was supported by a Presidential Young Investigator grant administered by the National Science Foundation, DMR-1234567.

References