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(Continuation see cover p. 4)

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The topology and geometry of infinite periodic surfaces

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Minimal surfaces / Liquid crystals / Crystallographic surfaces

Abstract. The use of space group stereohedra derived by Bashkirov as free boundaries result in a multiplicity of intersection-free (as well as self-intersecting) translationally periodic minimal surfaces of that space group. Surface solutions have differing tunnel networks and curvature, distinguished by their topology.

The exact geometry of these surfaces can be calculated by constructing a function which depends only on the surface normal vectors at flat points on the surface, and solving the Weierstrass equations. Translationally periodic surfaces of constant average curvature can be determined from the periodic minimal surface solutions.

Some examples of the various techniques for calculating the geometry and topology of these periodic surfaces are given.

1. Introduction

Infinite periodic minimal surfaces (IPMS) appear to provide useful descriptions of many natural structures and structural transformations, from cell membranes to crystals (both liquid and solid state) and electrostatic equipotentials (Andersson, 1983; Andersson et al., 1984; Hyde et al., 1984, 1986b; Hyde and Andersson, 1985, 1986a; v. Schnering and Nesper, 1987). It is becoming clear that related translationally periodic surfaces, surfaces of constant average curvature, are also naturally prevalent. These surfaces exhaust the list of stationary solutions to partitioning problems, i.e. they alone partition space into fixed volume fractions such that the surface area is stationary with respect to area perturbations (Grüter et al., 1986; Hildebrandt, 1985).

Unfortunately, progress in understanding these solid and liquid phases is hampered by the small number of translationally periodic surfaces known; to date about 20 examples of IPMS have been discovered (Schoen, 1970; Fischer and Koch, 1987; Lidin and Hyde, 1987). Apart from pioneering numerical work of Anderson (Nitsche, 1985; Anderson et al., to appear 1989), very little work has been done on periodic surfaces of constant average curvature (H surfaces) in three dimensions. [Examples of periodic H surfaces along a line were solved by Delaunay (see Hildebrandt and Tromba, 1985), while doubly periodic H surfaces confined between two planes have more recently been found by Lawson (1970).] It is clear that an infinite number of IPMS exist (Nagano and Smyth, 1978), and techniques for generation and classification of these surfaces necessarily involve topological ideas, as well as standard symmetry specification.

The link between topology and surface transformations is explored in the final section, leading to useful results for checking new periodic surface solutions. We show in the following sections how to systematically generate IPMS and H surfaces for any space group, and describe how to establish the detailed geometry and topology of the surfaces.

2. Geometry of periodic constant average curvature (H) surfaces

The geometry of translationally periodic surfaces is most neatly characterised in terms of the surface element (Flächenstück) bounded by an asymmetric unit of the space group of the surface, where the asymmetric unit uniquely defines the symmetry, just as kaleidoscopic cells characterise reflection groups (Hyde and Andersson, 1984). Suitable boundaries are those with arbitrarily curved faces and edges, *except where the face or edge actually coincides with a plane of mirror symmetry or symmetry axis* respectively. These conditions are almost met for every space group in $\mathbb{R}^3$ by the asymmetric units described by Bashkirov (1959). We impose a further (minor) constraint to those already considered by Bashkirov, namely that planar faces only occur for mirror planes. We call the resulting asymmetric units *Bashkirov stereohedra*. A surface bounded by a Bashkirov stereohedron may be analytically continued to form the infinite surface by simply adjoining Flächenstücke to form periodic surfaces of the space group defined by the stereohedron (Hyde, 1986).

For convenience we consider firstly minimal surface solutions to the free boundary problem formed by the Bashkirov stereohedron. These closed cell boundaries offer many possibilities for minimal surface solutions; unfortunately existence theorems for minimal surfaces on such free boundaries are few and far between. For tetrahedral cells, Smyth has shown that at most three disk-like solutions exist with a boundary curve in each face (Smyth, 1976). The multiplicity of more complex minimal surface solutions is not known, although it is clear that a large number of further minimal surface solutions exist.

A useful necessary property of minimal surface boundaries is Smyth's "balanced curve" criterion, which states that the sum of tangent vectors to the surface around the closed boundary curve on the stereohedral faces vanishes (Smyth, 1976). This criterion permits the sketching out on the stereohedral faces of the approximate boundary curve (i.e. successive edges intersected by the boundary). In the following section we show how the *topology* of the resulting IPMS can be determined from this approximate boundary configuration. Here we suggest that the detailed *geometry* of many IPMS can be calculated from this information alone.

The geometry of minimal surfaces is described almost everywhere by Weierstrass' equations, which give the cartesian coordinates of the surface in terms of generalised elliptic integrals (Nitsche, 1975):

$$x = \Re e \int_{\omega_0}^{\omega_1} (1 - \omega^2) \cdot R(\omega) \cdot d\omega$$

$$y = \Re e \int_{\omega_0}^{\omega_1} i \cdot (\omega^2 + 1) \cdot R(\omega) \cdot d\omega$$

$$z = \Re e \int_{\omega_0}^{\omega_1} 2\omega \cdot R(\omega) \cdot d\omega$$

where $\Re e$ refers to the real part of the integrals and i is the complex constant. The upper limit of the integral fixes the point on the surface whose coordinates are to be calculated, while the lower limit sets the orientation of the surface. The essential information regarding the geometry of the minimal surface is contained in the "Weierstrass function", $R(\omega)$, which is related to the Gauss map of the surface (Spivak, 1979).

These equations hold at all points on the minimal surface except flat points. At flat points the Weierstrass function is singular. We use this information to construct a suitable function to describe the geometry of periodic minimal surfaces. The proposed principle is simple: the Weierstrass function is the inverse of a polynomial which vanishes at all flat points. Each factor of the polynomial is raised to a power which is related to the topology of the surface, as described below.

Flat points on the surface are parametrised by the normal vector to the surface at the flat point. These vectors are parametrised within the complex plane by a real and an imaginary coordinate, formed by transforming the surface by its Gauss map, followed by stereographic projection onto the complex plane. The Gauss map transforms the surface onto a unit sphere. The intersection of the normal vector to the surface with the unit sphere – centred at the point to be mapped – corresponds to the Gauss map of the point. (Thus, for example, a horizontal portion of a surface is mapped onto a pole of the sphere.)

Stereographic projection from the north pole of the sphere, through the Gauss mapped point, onto a horizontal plane gives the (complex) coordinates of the point ($\omega = \sigma + i\tau$). The orthogonal axes of the plane correspond to the real and imaginary axes of the complex plane. [So that a horizontal portion of the surface, with an oriented normal vector pointing downwards, corresponds to $(\sigma, \tau) = (0,0)$, or $\omega = 0$.]

Provided that flat points of an IPMS lie on the Bashkirov stereohedral boundary, their normal vector and singularity order is easily determined from the stereohedral geometry, without recourse to the detailed boundary geometry of the minimal surface within the stereohedron.

We conjecture that the Weierstrass function is defined by the product:

$$R(\omega) = \frac{\xi}{\prod_{i=1}^{n} (\omega - \omega_i)^{\frac{1}{\beta_i + 1}}}$$

where ξ is a (real) scaling factor for the IPMS which determines the lattice parameters of the surface, the flat point normal vectors have complex plane coordinates ω_i and the order of the corresponding branch point is β_i. If ξ is complex, families of isometric surfaces are formed by varying its argument.

Flat points are most commonly located on stereohedral edges. The Gauss map of the complete surface in the vicinity of the edge is formed by concatenating the Gauss maps of all stereohedra which share this edge. If the concatenated Gauss map winds around the image of the surface at the edge more than once, the vertex is a flat point. If the map winds around n' times, the vertex forms an $(n' - 1)$th order branch point on the Riemann surface over the sphere. The reciprocal power in the Weierstrass function $(\beta_i + 1)$ is equal to n'.

An example is necessary to illustrate the simplicity of this technique. The quadrirectangular tetrahedron represents the Bashkirov stereohedron for cubic surfaces of space group $Pm\bar{3}m$, where all faces of the tetrahedron correspond to mirror planes. Taking this cell as a free boundary for a minimal surface, Smyth's balanced curve condition implies that all faces are traversed by the boundary of the surface. A simple balanced boundary is that shown in Figure 1, which represents the asymmetric unit of the IPMS known as the O,C–TO surface (Schoen, 1970).

Since a minimal surface must intersect its free boundary orthogonally (Grüter et al., 1986), the normal vectors of the O,C–TO Flächenstück at the boundary vertices must be parallel to the relevant tetrahedral edge direction vectors. Thus, the Gauss map of the surface boundary consists of great circles on the sphere, linking edge direction vectors of the quadri-

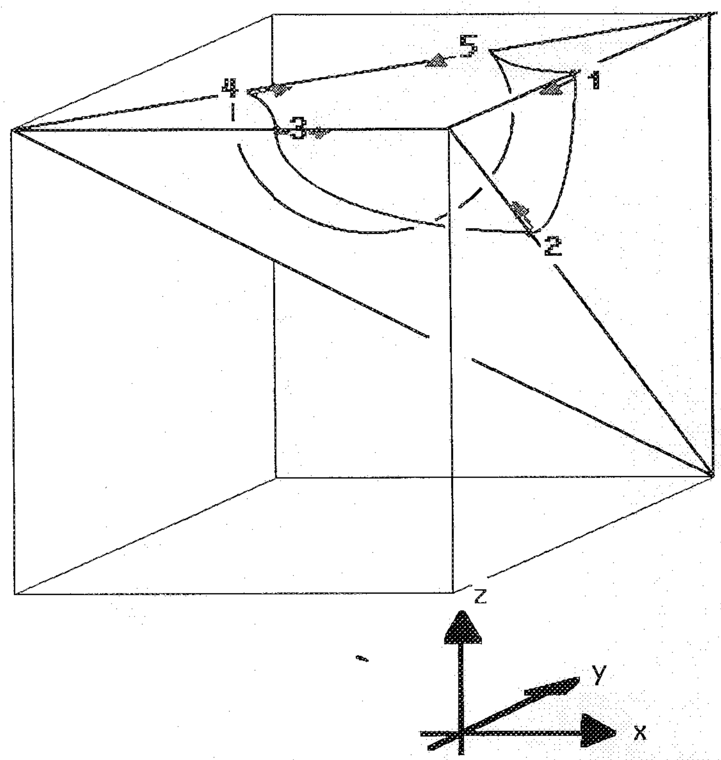

Fig. 1. A balanced curve (vertices 1, 2, 3, 4, 5) which represents a minimal surface solution to the free boundary quadrilateral tetrahedron, whose edges are shown as dark lines. The normal vectors to the minimal surface are indicated at the vertices. This boundary curve is a part of the O,C−TO surface discovered by Schoen (1970). The quadrilateral tetrahedron is the Bashkirov stereohedron for the cubic space group, *Pm*3*m*.

rectangular tetrahedron (whose sense is determined by orienting the surface consistently around its boundary).

The surface vertex normal vectors (in $\mathbb{R}^3$) are, as oriented in Figure 1,

$$(0,-1,0), \left(0,\ -\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right), \quad (1,0,0), \left(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0\right)$$

and

$$\left(-\frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}}, 0\right),$$

(ordered according to the vertex numbering shown in Fig. 1). Thus, vertices on the Gauss map of the O,C−TO Flächenstück correspond to these vectors.

The Gauss map of the surface onto the unit sphere and subsequent stereographic projection onto the complex plane is shown in Figure 2a and 2b. All vertices except vertices 2 and 3 subtend angles on the Gauss sphere equal to the dihedral angles at the edge. Vertices 2 and 3 subtend angles on

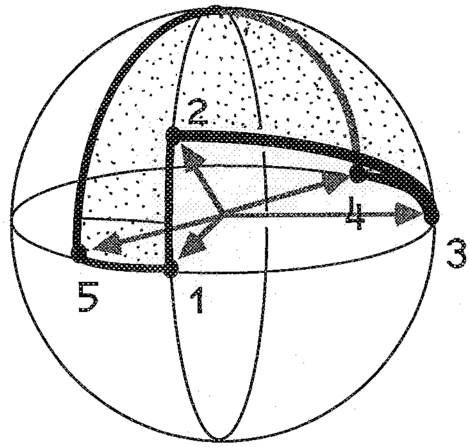

Fig. 2a. The Gauss map of the boundary curve in Figure 1. The surface normal vectors are projected onto the unit sphere. The mapped boundary vertices are indicated by large circles, numbered according to the scheme in Figure 1.

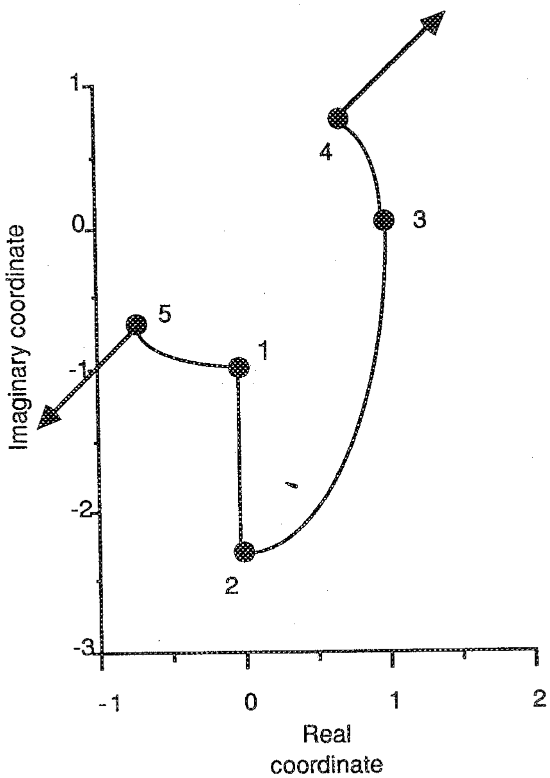

Fig. 2b. The complex plane representation of the boundary curve in Figure 1. This map is formed by stereographic projection of the Gauss map from the north pole of the unit sphere.

the Gauss sphere of $3\pi/2$ and $3\pi/4$ respectively. Since all faces are mirror planes, and the dihedral angles of the stereohedron at these vertices are $\pi/2$ and $\pi/4$ respectively, the concatenated Gauss map around points 2 and 3 subtend angles of 6π for both vertices, giving second order branch points (the Gauss map consists of three sheets in the vicinity of these points).

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Stereographic projection from the north pole of the unit sphere onto the complex plane (centred at the equator and parallel to the equatorial plane of the sphere) gives real and imaginary coordinates:

$$\sigma = \frac{x}{1-z} \quad \text{and} \quad \tau = \frac{y}{1-z}$$

respectively, where x,y, and z refer to the components of the $\mathbb{R}^3$ vectors, resulting in singularities of the Weierstrass function at:

$$\omega_1 = \left(0, \frac{1}{1-\sqrt{2}} \cdot i\right) \quad \text{and} \quad \omega_2 = (1, 0)$$

corresponding to vertices 2 and 3.

Reflection in the faces of the Bashkirov stereohedron results in other surface normal vectors. Since the O,C–TO Flächenstück bounded by a unit cell exhausts possible surface orientations, it is sufficient to determine flat point normal vectors on the surface contained within the parallelohedron (unit cell) derived by successive reflections in the faces of the stereohedron. The (cubic) parallelohedron derived from a quadrirectangular tetrahedral Bashkirov stereohedron consists of 48 such stereohedra (Fig. 3). The complete O,C–TO IPMS contains eighteen distinct flat point normal vectors, situated on three distinct circles centred at the origin of the complex plane (Fig. 4). In order to avoid the point at infinity in the complex plane (due to the singularity at the north pole of the Gauss sphere), it is necessary to re-orient the stereohedron. After some computation, the surface geometry can be obtained by substituting the Weierstrass function into the Weierstrass equations, from which the real space coordinates of the surface can be obtained by numerical computation of the elliptic integrals in Weierstrass' equations. The calculations are shown in detail in the Appendix.

Numerical estimation of the perimeter of the surface around the tetrahedron is extremely useful for characterising the surface area of the IPMS, which is a useful characteristic of the surface. If the area of the surface bounded by the stereohedron is A, and the length of the perimeter is l:

$$\frac{2 \cdot A}{l} = r$$

where r is the inradius of the stereohedron (Smyth, 1976). Unfortunately this result is only valid for tetrahedral stereohedra. Nevertheless, other boundaries can always be decomposed into tetrahedral simplices, for which the boundary length can be calculated once the real space coordinates of the surface are known.

The identification of flat points with symmetry elements of the space group (Nesper and von Schnering, 1985), means that flat points are usually

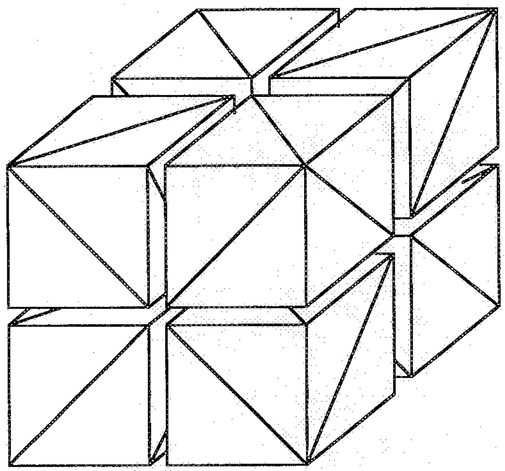

Fig. 3. A single lattice fundamental region for the space group $Pm\bar{3}m$, consisting of 48 quadrilateral tetrahedral Bashkirov stereohedra.

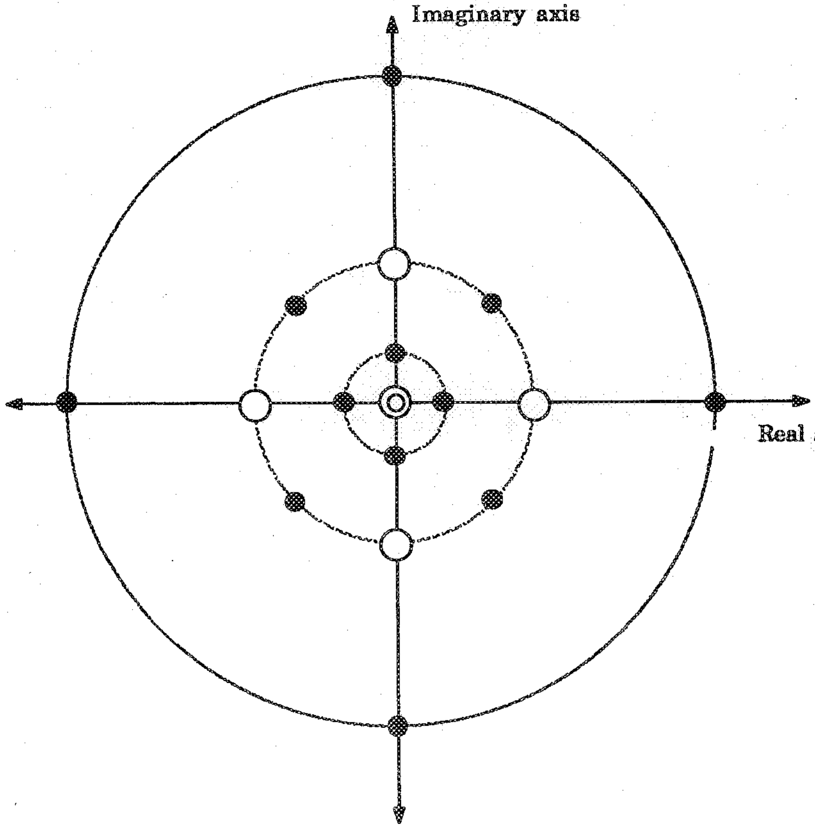

Fig. 4. The complement of 18 flat points with distinct normal vectors in the O,C–TO surface projected onto the complex plane, oriented as in Figures 1 and 2. The full circles represent flat point normal vectors equivalent to that at vertex 2 (Fig. 1); the open circles indicate all distinct flat point normal vectors due to symmetry operations on vertex 3. (The double circle at the origin indicates that both the origin and the point at infinity correspond to flat point normals.)

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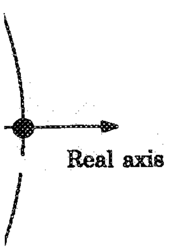

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located on edges of the stereohedron. However in some cases flat points are located within the stereohedron. With the help of topological techniques, outlined in the next section, the presence of internal flat point can be established. In some cases their normal vector is easily deducible from the geometry of the stereohedron (e. g. at the barycentre of the edge direction vectors), in other cases it is impossible without knowing the detailed surface geometry. In fact, such flat points can be oriented in any reasonable direction within the cell-giving rise to an infinite family of minimal surfaces (Lidin and Hyde, 1987; Lidin, 1988).

Other surfaces of constant average curvature can be geometrically determined from the related IPMS. The algorithm developed by Anderson (Anderson et al., to appear) permits numerical calculation of the geometry of these "*H* surfaces" once the geometry of the IPMS is known. Thus, using the techniques outlined in this section, along with Anderson's numerical algorithm, the geometry of periodic *H* surfaces can be calculated.

Work by Kenmotsu (1979) suggests that *H* surfaces can be generated by similar equations to the Weierstrass equations for minimal surfaces, using the same Weierstrass function as that for IPMS. If this is indeed the case, the method described here to obtain the Weierstrass function enables the computation of translationally periodic *H* surfaces, knowing only the approximate boundary morphology along the faces of the Bashkirov stereohedron.

3. Topology of periodic *H* surfaces

Topology plays an indispensible role in the study of surface structure. Apart from a fastidious desire to catalogue and index surfaces, it describes simply the morphology of structure: the connectivity of the tunnel networks on either side of the surface and the total curvature of the surface. Since periodic *H* surfaces are closely related to IPMS [up to "percolation" to spheres (Anderson et al., to appear)], we deal specifically only with IPMS.

It turns out to be most useful to describe IPMS by the Flächenstück bounded by their unit cell (the smallest portion of the surface which gives the entire IPMS under three lattice translation vectors). Under periodic boundary conditions, the Flächenstück is compactified, forming a finite surface (embedded in the three-torus). The genus of this compact surface efficiently characterises the surface topology.

This compactification procedure is most easily illustrated by an example. We take the simplest cubic IPMS, the *P* surface discovered by Schwarz (1890). The unit cell of this surface is a cubic parallelohedron (Fig. 5a). The lattice translation vectors of this surface link opposite faces of the cube. Under compactification, all points within a unit cell joined by lattice vectors are identified with each other ("glued") (Fig. 5b), resulting in a surface homeomorphic to a sphere with three handles (Fig. 5c). This

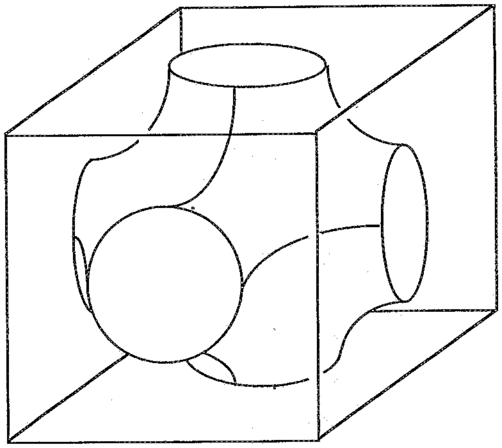

Fig. 5a. The fundamental region of the classical periodic minimal surface, the *P* surface. Note that this surface has space group $Im\bar{3}m$ (Hyde, 1986).

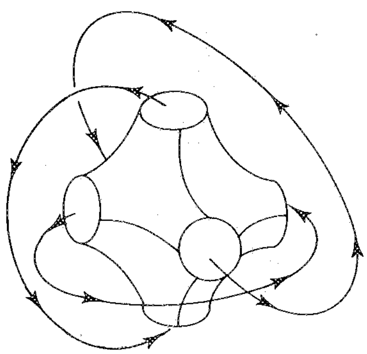

Fig. 5b. A fundamental region of the *P* surface, showing identification of surface elements linked by a lattice vector of the cubic network.

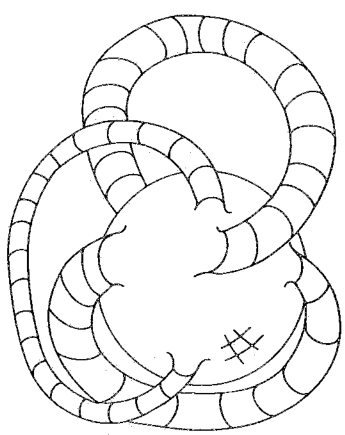

Fig. 5c. Abstract "gluing" of identified elements, giving a surface which is topologically equivalent to a sphere with three handles.

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surface has genus three (Goetz, 1970a), so we characterise the P surface as being an oriented surface of genus three and space group $Pm\bar{3}m$.

3.1. Orientability of minimal surfaces

Surfaces in three-dimensional space are most crudely topologically identified by their orientability characteristic, which distinguishes one- and two-sided surfaces. (The Möbius strip is an example of a one-sided or non-orientable surface.)

The mathematical characterisation of non-orientable minimal surfaces as "double surfaces", consisting of two overlapping leaves (each with equivalent normal vectors of opposite sense) leads to the possibility of continuously deforming non-orientable surfaces, separating the paired leaves and forming orientable surfaces (Sen, 1922). Thus minimal surfaces belong to the rare class of surfaces whose apparent orientability is not preserved under homeomorphisms.

3.2. Topology of IPMS and the labyrinth net

Since non-intersecting periodic minimal surfaces partition space into two connected regions, these surfaces can be structurally described by their tunnel geometry on either side of the surface, or their "labyrinth nets", described in detail elsewhere (Hyde and Andersson, 1984). Tunnels can be directed towards faces, edges or vertices of the parallelohedron in which the IPMS is embedded. Following Schoen (1970), we define the portion of an IPMS bounded by the unit cell as the *(lattice) fundamental region*.

If the fundamental region is considered as a polyhedron (as in Fig. 5), the topology of the Flächenstück can be determined by counting faces, edges and vertices of the polyhedron, using Euler's relation:

$$\chi = F - E + V \tag{1}$$

where χ is the Euler characteristic of the fundamental region and F, E and V are the number of faces, edges and vertices on the region (Goetz, 1970b). We take the relation between the genus and Euler characteristic of the (oriented) surface to be:

$$\chi = 2 - 2 \cdot g \tag{2}$$

where g is the genus. This is a matter of some flexibility [see, for example, Anderson et al. (to appear)], however we choose this definition on the grounds of simplicity: it is the standard topological definition; and self-consistency, since other relations result in inconsistent genera for the various techniques presented in this section.

Suppose that the fundamental region has t_2 tunnels directed toward the parallelohedral faces, t_1 tunnels towards edges and t_0 tunnels directed towards parallelohedral vertices. If all tunnels of the surface are capped with single faces, so that the fundamental region forms a closed polyhedron, it contains $(t_2 + t_1 + t_0)$ faces due to the caps. The number of edges and vertices around the caps must be equivalent (since an n-sided object necessarily contains n vertices); for simplicity we assume all tunnels intersect faces of the parallelohedron in a single edge, with a single vertex, while edge- and vertex-directed tunnels contain two and three edges and vertices respectively (Fig. 6).

In order to determine the topology of the compactified fundamental region (as in Fig. 5c), all caps must be removed and edge and vertex sharing with adjacent unit cells must be taken into account. Clearly, each face is shared with a single face of an adjacent parallelohedron, so that a half of the t_2 edges and t_2 vertices directed towards the parallelohedral faces belong to adjacent fundamental regions. If the edge-directed tunnels are slung over faces with a dihedral angle $2\pi/\alpha$ between them, a fraction of $(\alpha - 1)/\alpha$ of the $2 \cdot t_1$ vertices and a half of the $2 \cdot t_1$ edges are not included in the cell statistics. Similarly, if the three relevant dihedral angles of the vertices towards which t_0 tunnels are directed are $2\pi/\beta$, $2\pi/\gamma$ and $2\pi/\delta$, a fraction $(\beta - 1)/\beta$, $(\gamma - 1)/\gamma$ and $(\delta - 1)/\delta$ respectively of the $3 \cdot t_0$ vertices belong to adjacent regions. A half of the $3 \cdot t_0$ vertex-directed tunnel edges are not included in the statistics for the compactified surface.

If the Euler characteristic of the compactified fundamental region is χ, and the total number of faces, edges and vertices in the original capped polyhedron is N_2, N_1 and N_0, we have, using Euler's relation [Eq. (1)]:

$$\chi = [N_2 - (t_0 + t_1 + t_2)] - \left[N_1 - \left(\frac{t_2}{2} + \frac{2t_1}{2} + \frac{3t_0}{2}\right)\right]$$

$$+ \left[N_0 - \left\{\frac{t_2}{2} + 2t_1 \cdot \left(\frac{\alpha - 1}{\alpha}\right) + t_0 \cdot \left(\frac{\beta - 1}{\beta} + \frac{\gamma - 1}{\gamma} + \frac{\delta - 1}{\delta}\right)\right\}\right]$$

$$= [N_2 - N_1 + N_0]$$

$$- \left[t_2 + 2t_1 \cdot \left(\frac{\alpha - 1}{\alpha}\right) + t_0 \cdot \left(\frac{\beta - 1}{\beta} + \frac{\gamma - 1}{\gamma} + \frac{\delta - 1}{\delta} - \frac{1}{2}\right)\right].$$

If the genus of the original capped polyhedron is g', and the (required) genus of the compactified polyhedron is g, this expression simplifies using Eqs. (1) and (2) to give:

$$g = g' + \frac{t_2}{2} + \left(\frac{\alpha - 1}{\alpha}\right) \cdot t_1 + \left(\frac{\beta - 1}{\beta} + \frac{\gamma - 1}{\gamma} + \frac{\delta - 1}{\delta} - \frac{1}{2}\right) \cdot \frac{t_0}{2} \tag{3}$$

assuming the IPMS is orientable. (The genus of the capped fundamental region, g, is easily determined: it is equal to the maximum number of closed loops in the labyrinth net inside the polyhedron.)

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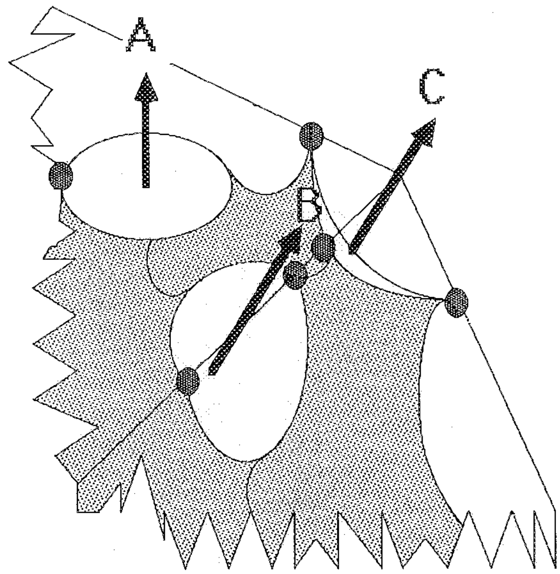

Fig. 6. Typical tunnel arrangements for translationally periodic surfaces: face-directed (A), edge-directed (B) or vertex-directed (C). In order to derive the topology of the surface we take the tunnels to have one, two or three edges and vertices (A, B and C respectively).

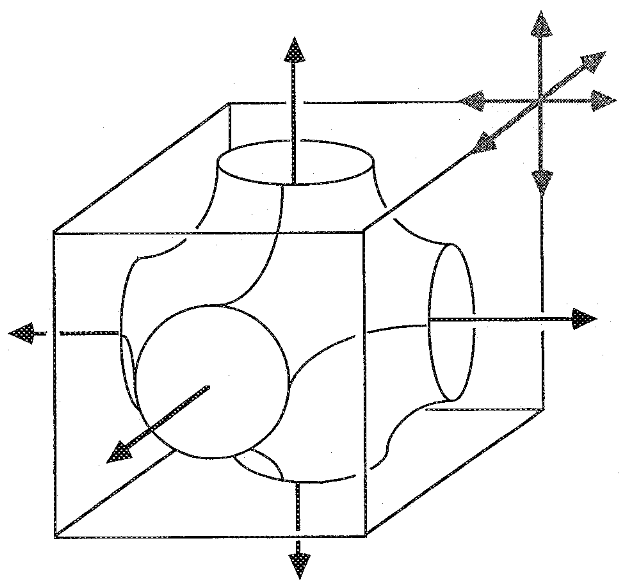

Fig. 7. The two interpenetrating simple cubic tunnel networks of the *P* surface.

For example, the interior labyrinth net of a fundamental region of the *P* surface consists of six edges radiating from the cube centre to the face centres, with a single net vertex at the cube centre (Fig. 7). Thus, the labyrinth net contains no loops (the capped fundamental region is topologically equivalent to a sphere, so that g' is zero) and six face-directed tunnels. Substituting these values into Eq. (3), we obtain a genus per fundamental region of:

$$g = 0 + \frac{6}{2} = 3,$$

equal to the value derived above.

Successive reflections of the O,C–TO Flächenstück (Fig. 1) in the quadrirectangular tetrahedral faces forms the fundamental region bounded by the cube shown in Figure 8a and 8b, which indicate both of the possible internal labyrinths. Neither labyrinth net contains a loop, so that the genus of the capped surface [g' in Eq. (3)] is again zero. From Figure 8a, the internal labyrinth contains two face-directed and twelve edge-directed tunnels (with dihedral angle $\pi/2$), giving a genus per fundamental region of ten. The tunnel system in Figure 8b contains six face-directed and eight vertex-directed labyrinths, so that the genus per fundamental region is again ten.

Note that the two inter-penetrating labyrinth nets are not geometrically equivalent for the O,C–TO surface [the surface is "unbalanced" (Fischer and Koch, 1987)]; a common possibility for periodic minimal surfaces lacking straight lines (Hyde and Andersson, 1984), and indeed, general periodic H surfaces. The labyrinth volumes on either side of the surface are also unequal (the Flächenstück in Fig. 1 cannot bisect the stereohedron into two equal volumes). This geometrical asymmetry between sides of an IPMS is nevertheless often overlooked in practice, where it has been widely (and falsely) assumed that the average curvature of a bicontinuous interface vanishes (giving zero average curvature) at an internal volume fraction of 50% (Jouffroy et al., 1982; Auvray et al., 1986).

3.3. Topology and the stereohedral geometry

Using the Gauss-Bonnet theorem, the genus of the surface can be calculated from the dihedral angles of the stereohedron alone, as long as the surface bounded by the stereohedron is simply connected.

This celebrated theorem relates the integral (Gaussian) curvature of a surface to the boundary angles, viz.

$$\iint_{\text{surface}} K\,ds = \int_{\text{boundary}} k_g\,dl + \left(2\pi - \sum_i \alpha_i\right)$$

where α_i are the exterior vertex angles of the boundary curve, K is the Gaussian curvature – integrated over the Flächenstück – and k_g is the geodesic curvature around the boundary (Goetz, 1970c). Assuming the stereohedron consists of planar faces, the boundary curves are plane lines of curvature, so that they are geodesic arcs, and the geodesic curvature is enus per funda-

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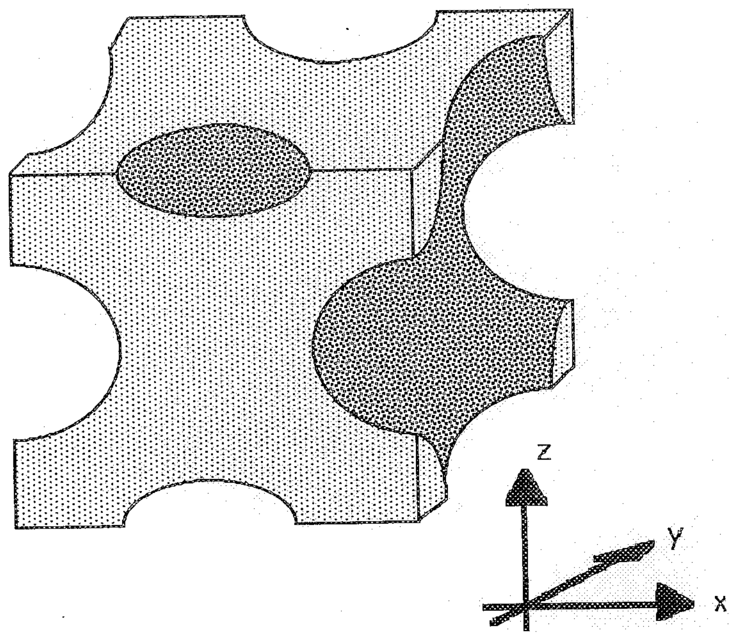

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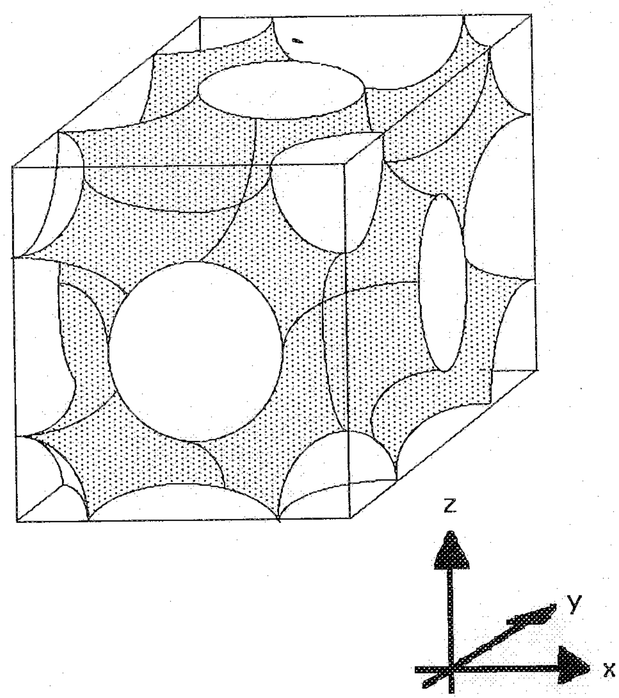

Fig. 8a, b. Alternative descriptions of a fundamental region of the O,C–TO surface, both bounded by cubes.

identically zero around the boundary. The vertex angles are simply the complement of the dihedral angles in the stereohedron traversed by the boundary. If N stereohedra form a parallelohedron, the integral curvature over a fundamental region of the IPMS is thus:

$$\iint_{\text{unit cell}} K\,ds = 2\pi \cdot N \cdot \left[1 - \sum_i \left(\frac{1}{2} - \frac{\delta}{2\pi}\right)_i\right] \tag{4}$$

where d_i are the internal dihedral angles. Euler's characteristic is directly related to the integral curvature:

$$\chi = \frac{\iint\limits_{\text{unit cell}} K\,ds}{2\pi} \tag{5}$$

(Hyde, 1986), so that the genus per fundamental region of an oriented IPMS is:

$$g = 1 - \frac{N}{2}\cdot\left[1 - \sum_i \left(\frac{1}{2} - \frac{\delta}{2\pi}\right)_i\right]. \tag{6}$$

Since N and δ_i are characteristics of the space group, formula (6) is easily determined.

Refering to the O,C–TO Flächenstück again, we see from Figure 1 that the dihedral angles subtended by the surface boundary are $\pi/2$, $\pi/2$, $\pi/4$, $\pi/2$, and $\pi/2$, and N is 48 (Fig. 3). Eq. (6) gives a genus per lattice fundamental region of the O,C–TO surface of ten – as found from the labyrinth net configuration.

For stereohedra containing non-planar faces, the algorithm is less useful, since the geodesic curvature does not vanish.

Since periodic H surfaces can be constructed from the Bashkirov stereohedron of the relevant space group, the vertex angle technique applies equally well to any H surface. Similarly, the labyrinth nets of H surfaces are unchanged – prior to percolation – from the "parent" IPMS (Nitsche, 1985), so that the technique for topological indexing of periodic surfaces outlined in the previous section is widely applicable to periodic H surfaces.

4. Merging geometry and topology of periodic surfaces

The link between curvature and topology of a surface implicit in the Gauss-Bonnet theorem can be exploited to provide a useful check on the Weierstrass function. It is instructive to consider the Weierstrass function as a Riemann surface on the sphere. The genus of a Riemann surface is related to the order and multiplicity of branch points and the number of sheets (s) of the surface by:

$$g = 1 - s + \frac{w}{2} \tag{10}$$

where w is given by:

$$w = \sum_i \beta_i \tag{14}$$

summing over all branch points in the fundamental region (Hopf, 1983). The mapping from the real space surface into the Riemann surface via Gauss' mapping is a homeomorphism over a fundamental region, so that the genus of the fundamental region of the surface is the same as the genus derived from the equation above. Furthermore, the Gauss-Bonnet relation establishes a link between the surface genus (via the Euler characteristic) and the number of sheets of the Gauss map, since an integral curvature of 4π covers the sphere once.

Rigorously:

$$\chi = \frac{\iint_{\text{unit cell}} K\, ds^2}{2\pi} = -2 \cdot s$$

where s is the number of sheets. (The negative sign is included to give a positive number of sheets, since the Gauss map covers the sphere "negatively", so that the winding number is negative.) Thus, if the surface is orientable:

$$g = 1 + s.$$

Comparing this equation with Eq. (10), the multiplicity of branch points,

$$\sum_i \beta_i = 4s$$

so that,

$$\sum_i \beta_i = -2 \cdot \chi. \tag{11}$$

This simple equation offers a useful check on the multiplicity and order of the flat points, since the topology of a fundamental region is easily determined from the labyrinth net or the stereohedral boundary vertex angles. For example, the genus per fundamental region of the O,C–TO surface was determined to be ten, giving a sum over all branch points of 36. It was shown earlier that these branch points are all second order. Hence, from Eq. (11) there must be 18 distinct flat points in the fundamental region of this IMPS, as found (see Appendix).

5. Conclusion

In this paper we have attempted to provide a rigorous guide to description of periodic surfaces of constant average curvature (H surfaces). Topological as well as geometrical concepts are indispensible to any discussion of these surfaces. The simplest way to describe and derive periodic H surfaces is in terms of the periodic minimal surface (zero average curvature) of the same symmetry and topology.

The translational periodicity of these surfaces is ensured by defining the surfaces as constant average curvature solutions of free boundaries which form asymmetric regions (stereohedra) of the crystallographic space groups. Suitable stereohedra are almost identical to those defined by Bashkirov. The detailed geometry of the minimal surface can be obtained by forming the Weierstrass function and determining the generalised elliptic integrals in the Weierstrass equations. This can be done without any prior knowledge of the surface shape except the approximate boundary geometry, which can be deduced from the balanced curve boundary conditions for minimal surfaces. Periodic H surfaces can then be generated using an algorithm developed by Anderson et al. (to appear), or, perhaps, using as yet unknown modified Weierstrass equations.

It is hoped that the techniques and applications presented here indicate the enormous undiscovered wealth of translationally periodic surface structures. For example, while only about twenty periodic minimal surfaces have been discovered, it is clear that an infinite number exist (Nagano and Smyth, 1978), and it is tempting to speculate that a countably infinite number exist for each space group!

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APPENDIX

Complex coordinates of the flat points of the O,C – TO surface

The singularities of the Weierstrass function correspond to the complex plane coordinates of those flat points belonging wholly to a fundamental region of the surface. Thus, flat points lying on the boundary of the parallelohedron are shared with each other to form a compactified Flächenstück.

The O,C – TO fundamental region shown in Figure 8b contains twelve internal flat points, with normal vectors pointing outwards from the cube centre to the edge mid-points. These vectors are:

$$\left(0,-\frac{1}{\sqrt{2}},\frac{1}{\sqrt{2}}\right),\left(0,\frac{1}{\sqrt{2}},\frac{1}{\sqrt{2}}\right),\left(-\frac{1}{\sqrt{2}},0,\frac{1}{\sqrt{2}}\right),\left(\frac{1}{\sqrt{2}},0,\frac{1}{\sqrt{2}}\right)$$

$$\left(0,\frac{1}{\sqrt{2}},-\frac{1}{\sqrt{2}}\right),\left(0,-\frac{1}{\sqrt{2}},-\frac{1}{\sqrt{2}}\right),\left(\frac{1}{\sqrt{2}},0,-\frac{1}{\sqrt{2}}\right),\left(-\frac{1}{\sqrt{2}},0,-\frac{1}{\sqrt{2}}\right)$$

$$\left(\frac{1}{\sqrt{2}},\frac{1}{\sqrt{2}},0\right),\left(\frac{1}{\sqrt{2}},-\frac{1}{\sqrt{2}},0\right),\left(-\frac{1}{\sqrt{2}},\frac{1}{\sqrt{2}},0\right),\left(-\frac{1}{\sqrt{2}},-\frac{1}{\sqrt{2}},0\right).$$

It also contains 24 flat points on the edges of the cube, straddling the cube vertices, with normal vectors along the cube directions. Each of these flat

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points is shared with three adjacent cubic cells, so that only six distinct flat point normals occur in the compactified region:

$$(0,0,1), (0,0,-1), (1,0,0),$$
$$(-1,0,0), (0,1,0), (0,-1,0).$$

These two types of flat point normal vectors can be projected onto the complex plane, as shown in Figure 4. The first of these flat point normal vectors points vertically upwards (indicated schematically by a point at the origin in Fig. 4), resulting in the point at infinity of the complex plane after stereographic projection from the north pole of the Gauss sphere. Since this is unsuitable for the Weierstrass function, it is necessary to re-orient the surface such that no flat points are directed vertically upwards. This is most simply achieved by rotating the sphere about the x-axis. Choosing an angle of rotation of $30°$, the vector coordinates are transformed by:

$$(x,y,z) \rightarrow (x, y\cdot\cos\{30°\} + z\cdot\sin\{30°\}, z\cdot\cos\{30°\} - y\cdot\sin\{30°\}).$$

Stereographic projection gives:

$$(\sigma,\tau) = \left(\frac{x}{1-z}, \frac{y}{1-z}\right)$$

resulting in complex plane branch points at:

$$\omega_1 = (0,-6.50);\ \omega_2 = (0,1.30);\ \omega_3 = (-1.83,0.91);\ \omega_4 = (1.83,0.91)$$
$$\omega_5 = (0,0.26);\ \omega_6 = (0,-0.77);\ \omega_7 = (0.44,-0.22);\ \omega_8 = (-0.44,-0.22)$$
$$\omega_9 = (0.52,0.45);\ \omega_{10} = (1.1,-0.95);\ \omega_{11} = (-0.52,0.45);\ \omega_{12} = (-1.1,-0.95)$$
$$\omega_{13} = (0,3.73);\ \omega_{14} = (0,-0.27);\ \omega_{15} = (1.0,0)$$
$$\omega_{16} = (-1.0,0);\ \omega_{17} = (0,0.58);\ \omega_{18} = (0,-1.73).$$

ordered as above.

Since all flat points form second order branch points (see main text), the Weierstrass function for the O,C−TO surface is a suitable combination of twelve of these branch points:

$$R(\omega) = \frac{\xi}{\prod_{i=1}^{12} (\omega - \omega_j)^{\frac{1}{3}}}$$

(where ξ is a real constant which determines the lattice parameter of the surface). The cartesian coordinates of the O,C−TO surface can then be determined by inserting this function into the Weierstrass equations. (Note that we choose twelve of the branch points, since the order of the Weierstrass function must be always equal to -4 in order to give the correct asymptotic form.)

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