

## Construction of candidate minimal-area space-filling partitions

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### ABSTRACT

Weaire and Phelan have shown that Kelvin tetrakaidecahedra are not the minimal surface partition of smallest area into regions of equal area. We develop a simple construction based on the Kelvin and the Williams partitions that generates periodic or quasiperiodic three-dimensional partitions, which are candidates for further improvements in surface area. It is important to distinguish between minimal-area structures under conditions of equal volumes and equal pressures.

The discovery of a space-filling structure composed of two types of cell of equal volume with a surface area less than that obtained by Kelvin (Weaire and Phelan 1994a) has stimulated further theoretical interest in the unsolved problem of how to partition three-space into equal volumes using surfaces of minimal area. The new structure may still not be optimal. Rivier (1994) has drawn attention to the large family of Frank–Kasper crystals, the duals of which are candidates for smaller-area structures. In the present letter we clarify some of these issues, and describe how further families of structures may be generated. It remains to be seen whether the surface area of these structures can be minimized without topological changes.

The type of problem considered by Weaire and Phelan was as follows.

(A) *All cells are of equal volume and the surface area is minimized*

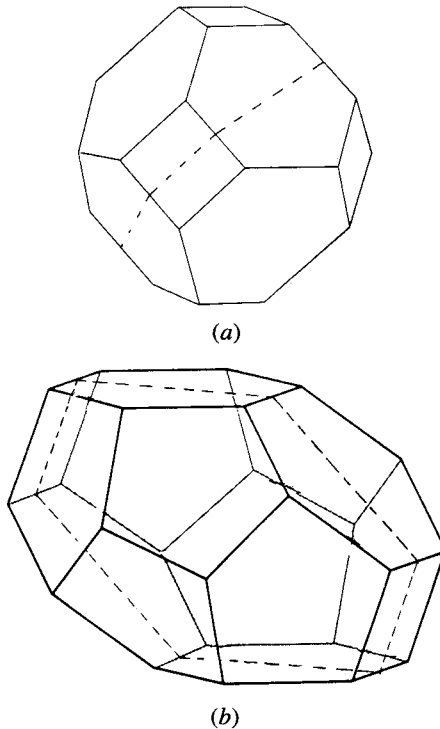
In general, we can specify only the volumes *or* the pressures of cells. The pressure difference between two cells is given by the surface tension times the derivative of total surface area with respect to the difference of their volumes.

Case (A) is realizable in the laboratory, but it would be more convenient to stipulate the following.

(B) *All cells have equal pressure and the surface area is minimized*

In this case, the mean curvature of each wall of each bubble is zero. Physically, zero curvature implies that there is no diffusion of gas across walls because pressures are equal; so the partition is stable against diffusion. In the trivial special case in which the cells are all identical and are related by translations of a lattice, their pressures are equal. Kelvin's solution of regular tetrakaidecahedra (fig. 1 (a)) falls into the following category.

Fig. 1



(a) Kelvin tetrakaidecahedron and (b) Williams cell (tetrakaidecahedron): (---), plane of the two-dimensional projections, corresponding to the bold hexagons in figs 2 and 3.

(C) *All cells have equal volume and pressure, by virtue of translational symmetry, and the surface area is minimized*

However, the non-symmorphic space groups allow a further possibility, in which cells are related by a translation and rotation so that they are identical but with different orientation as follows.

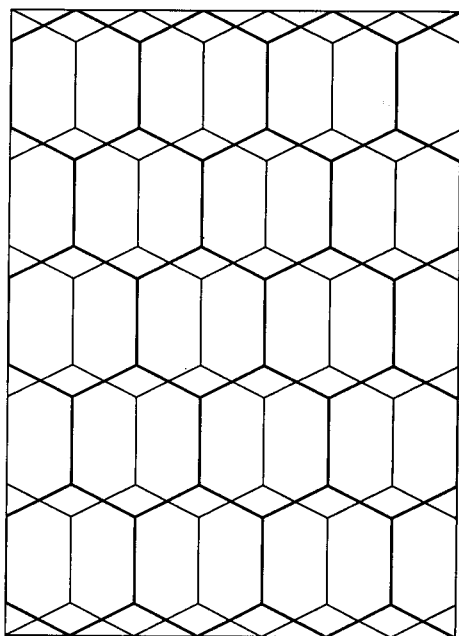
(D) *All cells have equal volume and pressure by virtue of translational and rotational symmetry, and the surface area is minimized*

The Williams (1968) cell falls into this category (fig. 1 (b)).

Some earlier writers refer to 'minimal froths' without defining which of the above they mean. Kusner (1992) deals with category (A) above, while Rivier (1994) wrongly associates both (A) and (B) with the work of Weaire and Phelan, the structure of which has two inequivalent types of cell and cannot satisfy both conditions. In fact, this work was devoted entirely to category (A).

Can we abandon (A) in favour of (B) and adjust a structure like that of Weaire and Phelan to satisfy the latter? At first this question seems trivial, but it is not. The pressure difference between the two inequivalent cells is proportional to the local curvature of the faces which separate them, which retains the same sign as the pressure is varied (R. Phelan 1994, unpublished), and cannot be reduced to zero, without topological changes. An argument of Sire (1994) shows that, for polyhedra with regular polygonal faces, the mean curvature depends only on the number of faces, while numerical simulations of Glazier (1993) indicate that the growth rate of a bubble (which is

Fig. 2



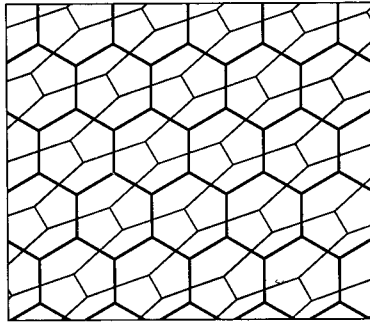
Two-dimensional vertical projection of half-plane of Kelvin tetrakaidecahedra  $K\uparrow$ : (—), downward-pointing vertices; (---) upward-pointing vertices. Each half-cell contains two quadrilaterals and two hexagons.

equivalent to the pressure difference between it and its neighbours, and hence its mean curvature) depends both on the number of faces and on their detailed topologies. Thus it appears nearly certain that partitions consisting of cells with differing numbers of faces cannot have uniform pressure. Partitions with similar numbers of faces but which lack uniform detailed topology may have uniform pressures, but we do not know of any.

We now develop a strategy to generate further candidate structures. They satisfy the necessary topological conditions (a cellular structure, with fourfold vertices), but in most cases we cannot say whether they survive area minimization without topological changes. During such minimization, all free parameters of the lattice should be varied, as well as the internal coordinates of the unit cell.

The Kelvin structure is b.c.c., with the cell shown in fig. 1(a). The cell can be divided in two on a plane perpendicular to the 110 axis (broken line in fig. 1(a)). The result is a half-layer, which (projected into the plane) consists of two parallel semiregular lattices of hexagons of long and short sides, displaced from each other by one half of the lattice spacing (fig. 2). One such half-layer has unconnected half-faces pointing up (light lines) while its partner has them pointing down (bold lines) (see fig. 2). We can perform a conformal transformation, such that each hexagon becomes regular in both lattices. In this case we denote the first half-layer by  $K\uparrow$ . Its mirror reflection we denote by  $K\downarrow$ . Thus the simple Kelvin partition is  $(K\uparrow K\downarrow)^n$ . Note that each  $K$  half-layer has a preferred orientation in its own plane (perpendicular to the displacement between the lattices). A rotation of the lattice by an angle  $\theta$  may be designated  $K(\theta)$ . If  $\theta = 0^\circ, 60^\circ$  or  $120^\circ$  the hexagonal lattices correspond and may be reconnected to form

Fig. 3



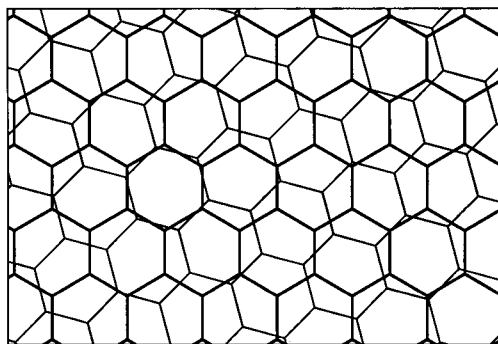
Two-dimensional vertical projection of half-plane of Williams tetrakaidecahedra  $W\uparrow$ : (—), downward-pointing vertices; (---), upward-pointing vertices. Note that both hexagonal lattices cannot be made regular. Each half-cell contains two quadrilaterals and two hexagons.

tetrakaidecahedra. If we have a sequence  $K\uparrow(0)K\downarrow(60)K\uparrow(120)K\downarrow(180)\dots$ , we have a regular periodic lattice composed of twisted Kelvin cells (Weaire and Phelan 1994b). Such cells, which occur in thin sandwiches of foam, have four quadrilaterals, six hexagons and four pentagons and have a chirality, if we do not allow reflection in the 110 direction. However, we are free to choose the orientation of each half-layer independently. Sequence  $K\uparrow(\theta)K\downarrow(\theta)$  give a layer of Kelvin tetrakaidecahedra,  $K\uparrow(\theta)K\downarrow(\theta + 60)$  (or  $K\downarrow(\theta)K\uparrow(\theta + 120)$ ) give right-handed twisted Kelvin cells, and  $K\uparrow(\theta)K\downarrow(\theta + 120)$  (or  $K\downarrow(\theta)K\uparrow(\theta + 60)$ ) give left-handed twisted Kelvin cells. Any sequence  $K\uparrow(\theta)K\downarrow(\theta + n_1 60)K\uparrow(\theta + n_2 60)K\downarrow(\theta + n_3 60)\dots$  is admissible and generates candidates for our category (C). If the sequence  $\{n_i\}$  has additional symmetry, for example,  $\{1, 2, 3, \dots\}$ , then we have an example of case (D).

Williams (1968) proposed a structure which A. Kraynik (1994, unpublished) has shown is stable under area minimization, contradicting the claim of Ross and Prest (1986). It is of type (D) with two equivalent cells (fig. 1 (b)) whose centres lie on a b.c.t. lattice but have perpendicular orientations in consecutive layers perpendicular to the  $c$  axis. Again, we can divide the Williams cell into two halves (broken line in fig. 1 (b)) to create a sheet of irregular hexagons, which we project on to the plane (fig. 3; the bold hexagons correspond to the broken line). Williams constructed his lattice by making topological changes in an isolated Kelvin cell and then packing the resulting cells. We use our hexagonal lattice notation to generate the structure. Consider the lattice shown in fig. 2. Leave the bold lattice unchanged and perform a T1 (side swap), on the parallel light lines at the centre of each hexagon. As before, we now have two hexagonal lattices: one regular and the other of elongated hexagons (fig. 3). We cannot make this second lattice regular by conformal transformation in a flat space, unless we destroy the regularity of the first, since the diagonal length of a hexagon is not equal to its height. Only in a curved space, where  $\cos(30^\circ) = 0.75$ , do both lattices become regular. We call the lattice with the regular hexagons upward pointing  $W\uparrow$ , and the lattice with the unconnected regular hexagons downward pointing  $W\downarrow$ . As before, we have three allowed orientations of the lattice, at  $n60^\circ$ . The normal Williams cell consists of repetitions of  $W\uparrow(\theta)W\downarrow(\theta)$ . A second T1, applied to the first lattice, regenerates the K lattices.

Alternatively, we may generate the Williams cell directly from the Kelvin tetrakaidecahedron by an elementary topological change (Schwartz 1964) applied to all

Fig. 4



Two-dimensional quasiperiodic half-plane  $G(45^\circ)\uparrow$ : (—), downward-pointing vertices; (—), upward-pointing vertices.

the quadrilateral faces perpendicular to the 001 direction, rotating them in successive layers towards the 110 and  $1\bar{1}0$  lines, respectively. The construction shows the relation between the b.c.t. lattice and the b.c.c. lattice of the Kelvin structure. However, the lattice of the structure as a whole is simple tetragonal.

As before, we can combine W half-planes of different orientations and W and K half-planes. However, because of the broken symmetry,  $W\downarrow(\theta)$  must be followed by  $W\uparrow(\theta)$ . However,  $W\uparrow(\theta)$  may be followed by any other  $\downarrow$  half-plane.

The sequence  $W\uparrow(\theta)W\downarrow(\theta)$  yields Williams polyhedra with two square, eight pentagonal and four hexagonal faces.  $W\uparrow(\theta)W\downarrow(\theta \pm 60^\circ)$  yields the barrel with 12 pentagonal and two hexagonal faces (in our hypothetical curved space with  $\cos(30^\circ) = 1.5$ , the barrel is space filling).  $W\uparrow(\theta)K\downarrow(\theta)$  yields four squares, four pentagons and six hexagons.  $W\uparrow(\theta)K\downarrow(\theta \pm 60^\circ)$  yields two squares, eight pentagons and four hexagons, but in a different arrangement from that of the Williams cell (different detailed topology). This cell, like the twisted Kelvin cell, has two chiralities. All these structures are entirely tetrakaidecahedral and hence it may be possible to construct partitions of equal pressure using combinations of them.

If we are willing to abandon our requirement that we have only one cell type, we can generate an infinite family of periodic and quasiperiodic structures starting with our two simple hexagonal lattices. If we misalign two regular hexagonal lattices by an angle  $\phi$ , we obtain a tiling of the plane,  $G(\phi)$  with multiple cell types (there are 11 possible hexagonal unit-cell topologies). If  $(\tan \phi)/3^{1/2} = p/q$  in lowest terms, where  $p$  and  $q$  are integers, then the lattice  $G(\phi)$  is periodic with period  $p$  in the direction of  $0^\circ$  and  $q$  in the direction  $90^\circ$ . If  $(\tan \phi)/3$  is irrational, the lattice  $G(\phi)$  is quasiperiodic (fig. 4). In either case, because the lattice consists of two regular hexagonal grids, we can combine  $G(\phi)\uparrow(\theta)$  with  $G(\phi')\downarrow(\theta \pm n60^\circ)$  and  $G(\phi)\downarrow(\theta)$  with  $G(\phi')\uparrow(\theta \pm n60^\circ)$  for any  $\phi$  and  $\theta'$ . Since the sequences  $\{\phi_i \in [0, 360]\}$  and  $\{n_i \in 1, 2, 3\}$  are arbitrary, we have a mechanism to generate large families of periodic or quasiperiodic minimal partitions. Again, the existence of the sequence need not imply the stability of the topology under minimization.

The next step should be to test these partitions under minimization, since their topological stability is difficult to predict.

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