COMPARING THE WEAIRE-PHELAN EQUAL-VOLUME FOAM TO KELVIN'S FOAM

ROB KUSNER AND JOHN M. SULLIVAN

1. Introduction

The problem of partitioning space into equal-volume cells, using the least interface area, was considered in 1887 by Sir William Thomson, Lord Kelvin [Kel]. His proposed solution yields a foam with cells of a single shape, tiling space by the translations of the body-centered cubic lattice. In 1993, Denis Weaire and Robert Phelan [WP] proposed a new equal-volume foam with two different cell shapes, which uses less area according to their computer experiments with Ken Brakke's `evolver` [Bra].

Mathematically, one difficulty is that neither foam can be described explicitly; even their existence is troublesome. In this note, we will examine these two foams, showing that the Weaire-Phelan foam is in fact more efficient than the Kelvin foam, and we will describe some other interesting candidate foams. More mathematical details, including a proof of existence for the Kelvin foam, are forthcoming in [AKS].

A *partition* of space is a division of $\mathbb{R}^3$ into disjoint cells. We are mainly interested in the surfaces forming the interface between the cells. The partitions we consider will be periodic with respect to some lattice, with some number n of cells in each periodic domain; thus they could be viewed as partitions of a quotient three-torus into n cells. Fixing the volume of each cell to be V, we want to minimize the *cost* of the equal-volume partition, defined scale-invariantly to be $\mu := A^3/V^2$, where A is the average interface area per cell. (Note that A is really half the boundary area of a typical cell, since each interface is shared by two cells.) If we scale to make $V = 1$, the case of unit-volume cells, then our cost is simply the cube of the total surface area in a periodic domain, divided by n^3.

If we start with some partition, perhaps polyhedral, and let it relax until the cost is a minimum, at least among nearby partitions, then the resulting stable partition should exhibit the geometry of a cluster of soap bubbles. Thus a stable partition should follow the rules recorded by Plateau [Pla] in 1873 for such clusters, and proved by Jean Taylor [Tay] in 1976 for a certain mathematical model (due to Fred Almgren) of compound bubbles.

These *Plateau rules* state that the interfaces are smooth surfaces of constant mean curvature, except where they meet in threes (at equal 120° angles) along smooth arcs. These arcs are, furthermore, allowed to come together (four at a time) at isolated points, where the configuration is tetrahedral; but no other singularities are allowed. The allowed singularities are observed for instance in a cluster of three

Date: (Received January 9, 1996; Accepted July 24, 1996).

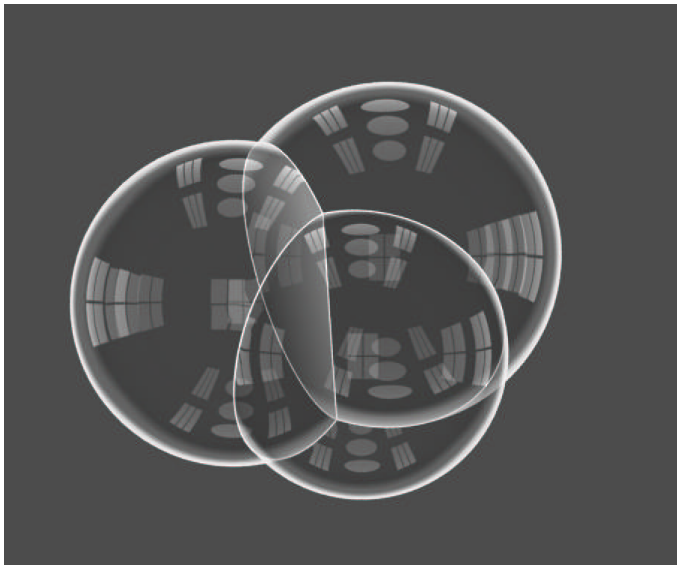


Figure 1. This triple bubble in space exhibits the Plateau singularities: smooth surfaces meet along triple-junction curves at 120° angles, and these junctions come together at tetrahedral points.

or more soap bubbles, as in Figure 1. The mean curvature of each surface is simply the pressure difference between the two cells on either side; this implies for instance that the three mean curvatures around a triple junction sum to zero.

We can view these rules as having a geometric part (about curvatures and equal angles) and a combinatorial part: that cells should meet along edges in threes, and at corners in fours, tetrahedrally. This combinatorics is the same as is observed generically in Voronoi partitions. Given a collection of sites in space, we define the *Voronoi cell* [Sen, OBS] for each site to be the region consisting of points closer to that site than to any other. Figure 2 shows an example in the plane. In space, the boundary between two adjacent cells in the partition is a polygonal piece of the plane perpendicularly bisecting the segment between the two sites. These bounding polygons meet along segments equidistant from three sites, which terminate at vertices equidistant from four sites. The Voronoi partition of a symmetric collection of sites will share its symmetry.

This similarity in combinatorial structure suggests we might find foams as relaxed Voronoi partitions. We specify certain sites and compute their Voronoi partition to get polyhedral cells in the right combinatorial structure; then we can follow mean curvature flow (with volume constraints) toward a stationary foam satisfying the geometric Plateau rules. This idea was implemented numerically at the Geometry Supercomputer Project in 1988, using Sullivan's `vcs` software [Sul] to compute Voronoi partitions in three dimensions, and Brakke's `evolver` to relax them to foams. Some results appeared in the movie "Computing Soap Films and Crystals",

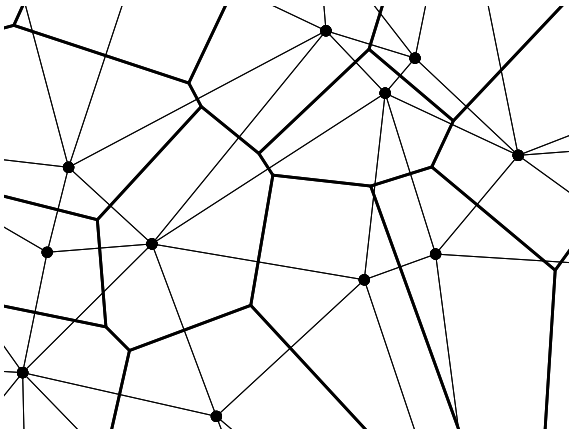


Figure 2. Sites in the plane (marked with dots) together with their Voronoi partition (heavy lines). The thin lines are the dual Delone triangulation, connecting sites with adjacent Voronoi cells.

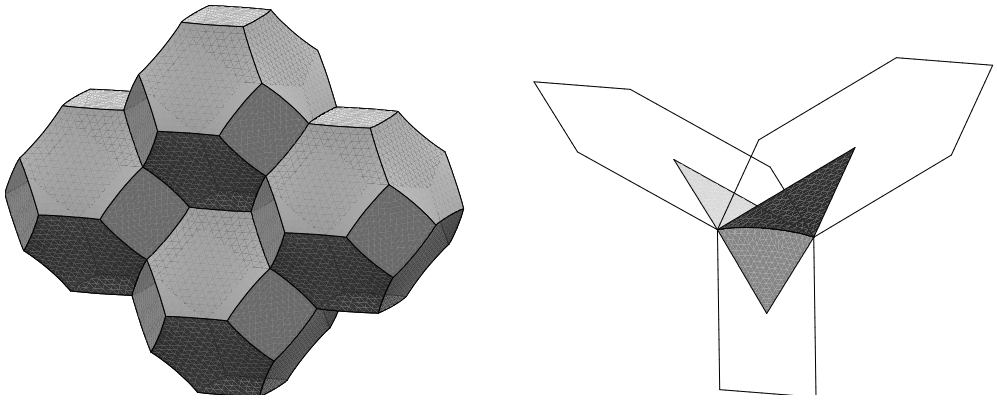
produced by Almgren, Brakke, Sullivan and Taylor, and published in [Alm]. Those experiments found no foams better than Kelvin's. But Weaire and Phelan knew of an interesting pattern (often called A15) arising in chemical clathrates, and used the same pair of programs to find that the corresponding foam did have lower cost.

There is not enough mathematical theory for mean curvature flow with triple junctions to know in general when this Voronoi procedure for constructing foams really works. Certainly topological or combinatorial changes may occur if the relaxation flow proceeds far enough; such singularities can lead to nonuniqueness for the continued mathematical flow [ACI]. However, all the foams we will consider will be constructed in this way, evidently without such topological changes. In each case, the Voronoi sites determine a certain pattern of combinatorics and symmetry, and presumably there is a unique relaxed foam in this pattern, close to the one we observe computationally.

The cells in a Voronoi partition do not in general have equal volumes. The `evolver` can adjust the volumes towards the desired targets as the numerical relaxation proceeds. But mathematically it is helpful to start with the correct volumes. A *weighted* Voronoi partition is a generalization in which different weights on the various sites change the relative sizes of the cells; each interface plane is moved away from the site of higher weight. With appropriate weights, the initial Voronoi cells will have the desired volumes, and there is less chance that the mean curvature flow will cause combinatorial changes.

2. The Kelvin foam

Kelvin described his foam as a relaxation of the Voronoi partition for the body-centered cubic lattice `bcc`, whose cells are congruent truncated octahedra. We will take this `bcc` lattice to be generated by $\texttt{cyc}(2, 2, -2)$, by which we mean the three



(a) (b)

Figure 3. Four cells in the relaxed Kelvin foam (a), and one fundamental piece (b), consisting of a fourth of one square and sixths of two hexagons, the region near a particular triple edge. The outlined polygons in (b) show the original locations of nearby triple edges to help locate the figure; of course in the relaxed foam these would also bend.

vectors given by cyclic permutations of these coordinates. This lattice consists of the cubic lattice $\mathsf{cub} = 4\mathbb{Z}^3$ and its translate by $(2, 2, 2)$. The Voronoi cell around the origin touches fourteen others: the six nearest neighbors in the cubic lattice, and eight along body diagonals. (Kelvin called this cell a tetrakaidecahedron because of its fourteen faces. Of course, there are many other 14-hedra, such as the one we encounter in the next section; this cell is best described as the (Archimedean) truncated octahedron.) The 24 vertices of this cell are the points $\mathsf{cyc}(0, \pm 1, \pm 2)$ and $\mathsf{cyc}(\pm 2, \pm 1, 0)$. This unrelaxed foam has cost $\mu = \frac{27}{128}\left(30\sqrt{3} + 37\right) = 18.7653\cdots$.

The Voronoi partition of course has the full group of symmetries of the lattice. We will call this group G_0; it is the crystallographic group $Im3$. It is generated by the bcc translations and by sign changes and permutations of the coordinates. This group acts transitively on (oriented) edges of the Voronoi partition (or the Kelvin foam). In particular, all the edges are congruent.

We will say, of any partition which has this same combinatorics and symmetry, that it is in the *Kelvin pattern*. In particular, when we relax the polyhedral partition, the symmetry is preserved, so the resulting Kelvin foam is in the same pattern. As the foam relaxes, the vertices are fixed by symmetry. The square faces remain in their mirror planes, although the edges bow out within these planes. The diagonals of the hexagons remain fixed along axes of rotational symmetry, while the hexagons become shaped like monkey-saddles. (The diagonals of the squares also lie along axes of two-fold rotational symmetry.)

Physically, it is easy to see that soap film in the Kelvin pattern will relax (moving only slightly, as just described) to the foam shown in Figure 3(a). Mathematically, we can also prove the existence and uniqueness of such a foam [AKS].

Consider now the piece of the foam nearest to a particular triple-junction edge (as in Figure 3(b)). It includes a quarter of one square and sixths of two hexagons, and its boundary is along axes of 180° rotational symmetry. This unit will generate the entire foam under these rotations; it also has further four-fold symmetry given by a pair of mirror planes. The boundary of the unit can be thought of as three V-shaped planar wires, welded together at their ends. There is a sheet of the foam surface hanging on each wire, and these sheets meet along a curved triple junction.

We can give a lower bound for the area of this (or any partition in the Kelvin pattern) by a *slicing argument*. We will slice the fundamental unit just described by planes perpendicular to the original edge. Each slicing plane meets the three boundary wires of the unit, and the slice of the surface is Y-shaped, connecting these three points. It thus has at least as much length as the Steiner tree on these points. Furthermore, the area of the whole unit is at least the integral of the lengths of the slices. In fact, because the boundary wires are linear, the Steiner trees in the parallel planes are similar to one another, so it is easy to compute this lower bound explicitly [AKS]. We find that the cost of the Kelvin foam is bounded below by $\mu > \frac{27}{16}\left(\sqrt{3/2}+1\right)^3 > 18.5816$. (Experiments with the `evolver` show partitions in the Kelvin pattern with cost just under 18.67582; presumably this is close to the true cost of the Kelvin foam.)

3. The Weaire-Phelan foam

Certain metals, like the β-form of tungsten or a chromium-silicon alloy, crystallize with atoms in a close packing called A15. This includes the sites of the `bcc` lattice together with half of its Voronoi corners: the points $\texttt{cyc}(0, \pm 1, \pm 2)$ and their translates by `cub`. Weaire and Phelan based their foam on the pattern of the Voronoi cells for this A15 packing. The pattern has a (pentagonal) dodecahedron centered at each `bcc` lattice site, and a certain 14-hedron around each of the other sites, as seen in Figure 4. This 14-hedron might be viewed as a "$\frac{6}{5}$-fold unwrapping" of a pentagonal dodecahedron, since it has two opposing hexagon faces and two belts of six pentagons surrounding these hexagons.

The symmetries of the pattern (crystallographic group $Pm\bar{3}n$) form a subgroup G of index two in G_0. This subgroup is generated by the `cub` lattice translations, cyclic permutations and sign changes of the coordinates (geometrically, three-fold rotation and mirror symmetries), together with a motion which combines translation by $(2, 2, 2)$ with an odd permutation of the coordinates (geometrically, translation and an order-four rotation about a coordinate axis).

In one translational unit cell for the `cub` lattice $4\mathbb{Z}^3$ (whose volume is $4^3 = 64$) we have two dodecahedra and six 14-hedra. For an equal-volume partition, each cell should have volume $V = 8$. Up to symmetry in the pattern, there are two kinds of cells, three kinds of faces (hexagons, pentagons on dodecahedra, and other pentagons), four kinds of edges, and three kinds of vertices (those touching zero, one, or two hexagons).

Any dodecahedron around the origin with this symmetry will have eight corners at $(\pm a, \pm a, \pm a)$, which are the vertices touching no hexagons, and twelve corners

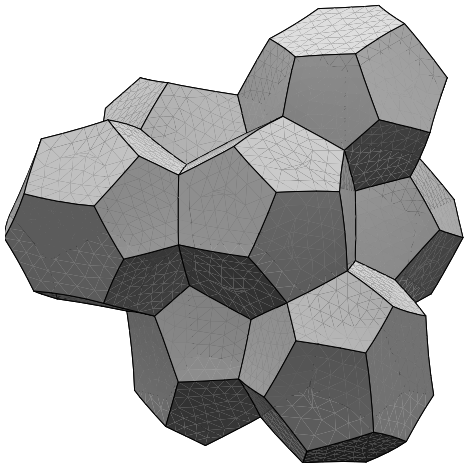


Figure 4. Eight cells, forming a fundamental unit of the Weaire-Phelan foam. In front, we see a dodecahedron with slightly higher pressure than the neighboring cells. These are 14-hedra, with two parallel hexagonal faces, stacked in columns in the three coordinate directions.

$\mathtt{cyc}(0, \pm b, \pm c)$, the ones touching one hexagon. We take $0 < b < a < c < 2$ to fix orientation. (Choosing instead $b > c$ would give the same pattern rotated by $90°$, or translated by $(2, 2, 2)$.) These parameters are not fixed by the symmetry. We will not try to describe the actual least-area foam in this pattern, but only an equal-volume polyhedral partition, the appropriately weighted Voronoi partition.

The pentagonal faces are planar if $(a - c)^2 = a(a - b)$. Then their area is $\left(a\sqrt{a-b} + (a+b)\sqrt{a}\right)\sqrt{2a-b}$. The dodecahedron's volume is $4a(2ac + bc - ab)$.

To examine the other cells, write an arbitrary point $(1+p, 0+q, 2+r)$ as $[p, q, r]$. Then the cell near $(1, 0, 2) = [0, 0, 0]$ has dodecahedral neighbors around $[-1, 0, \pm 2]$, $[1, \pm 2, 0]$, and other neighbors around $[\pm 2, 0, 0]$, and $[1, \pm 1, \pm 2]$ and $[-1, \pm 2, \pm 1]$. Since we know the vertices of the dodecahedra in terms of a, b, c, we can list the vertices this cell shares with its dodecahedral neighbors:

$$[1 - a, \pm(2 - a), \pm a], [1 - c, \pm(2 - b), 0], [1, \pm(2 - c), \pm b],$$

and

$$[a - 1, \pm a, \pm(2 - a)], [c - 1, 0, \pm(2 - b)], [-1, \pm b, \pm(2 - c)].$$

The remaining vertices (those touching two hexagons, and four of the 14-hedra), are actually fixed by the symmetries: the vertex between the cells around $[0, 0, 0]$, $[2, 0, 0]$, $[1, 1, 2]$, and $[1, -1, 2]$ is at their center of mass $[1, 0, 1]$, so the vertices of our cell not listed above are $[1, 0, \pm 1]$ and $[-1, \pm 1, 0]$.

We now compute the areas of the faces of this cell not shared with dodecahedra. The face to the cell at $[2, 0, 0]$ is a planar hexagon, with area $4(2-c)b+2(2-c)(1-b) = 2(2 - c)(1 + b)$. The face to the cell at $[1, 1, 2]$ is a pentagon with vertices

$$[1, 0, 1],\ [1, 2 - c, b],\ [1 - a, 2 - a, a],\ [-1 + a, a, 2 - a],\ [-1 + c, 0, 2 - b].$$

This will be planar if $2b = c$. Making this assumption, we can divide it into one isosceles triangle of area $(1-a)\sqrt{6}$ and two congruent triangles of total area $a(1-b)\sqrt{6}$.

The foam within a unit cell of `cub` has two dodecahedra and six other cells, and thus has 24 dodecahedral faces, six hexagonal faces, and 24 of the other pentagonal faces. The area of these taken together is $8A$ where A is the average area per cell.

Under our assumptions of planarity, $4b = 2c = 3a$, and it is easy to check that each face is perpendicular to the line connecting the cell centers, so that our polyhedral foam is actually a weighted Voronoi partition on these centers, where the relative weighting between the `bcc` centers and other centers depends on c. Also, we compute that the area is $8A = 24 + 24\sqrt{6} + \left(12\sqrt{5} - 8\sqrt{6} - 6\right)c^2$, while the volume of the dodecahedron is $V_d = 4c^3$. To get an equal volume foam, we must take $c = \sqrt[3]{2}$, which gives $A = 3 + 3\sqrt{6} + \left(6\sqrt{5} - 4\sqrt{6} - 3\right) / \sqrt[3]{16}$ and $V = 8$. The cost ratio $\mu = A^3/V^2$ for this partition is then just under 18.57752.

We have thus shown that even this unrelaxed, polyhedral partition in the A15 pattern has less cost than any Kelvin partition. Experiments with the `evolver` give better partitions in this pattern, with cost just under 18.4871. Presumably there is a unique Weaire-Phelan foam in this pattern, with cost close to this value. The lower symmetry of the A15 pattern compared to the Kelvin pattern, however, leaves mathematical existence results and cost bounds out of reach.

4. Other possible foam structures

Because the edges of any foam meet at tetrahedral angles $\arccos(-1/3) \approx 109.47°$, which is close to the angle of a regular pentagon, there has been repeated speculation [Riv, Wil, Cox] that efficient foams would have pentagonal faces, unlike Kelvin's foam. Of course, using only pentagons, each cell would be a dodecahedron, and these do not tile Euclidean space. However, there is a large class of foams in which the faces are all pentagons or hexagons, as in the Weaire-Phelan foam.

There are only four types of polyhedra which have only pentagonal and hexagonal faces, with no adjacent hexagons. These are the dodecahedron, the 14-hedron we have already seen, and two more polyhedra, with 15 and 16 faces, again each including twelve pentagons. Chemists have observed many transition-metal alloys in which each atom has a Voronoi cell of one of these types (and thus, valence 12, 14, 15, or 16). These crystals are called *tetrahedrally close-packed* (TCP) structures [FK]. The same structures are also observed chemically in clathrates, like chlorine hydrates, with oxygen atoms at the Voronoi corners bonded by hydrogen along the Voronoi edges, forming cages in which large gas molecules sit (at the sites of the metal atoms in the first structure).

There are several dozen TCP structures observed by the chemists, and further infinite families can be constructed by mixing these: in fact, there seem to be three basic structures—A15, Z and C15—from which all the TCP structures can be made (see Figure 5). For each, the Voronoi partition can be relaxed to an equal-volume foam as before. For Z or A15 or any mixture of these, the foam seems to have cost less than that of Kelvin, with the cost decreasing as we approach A15; the

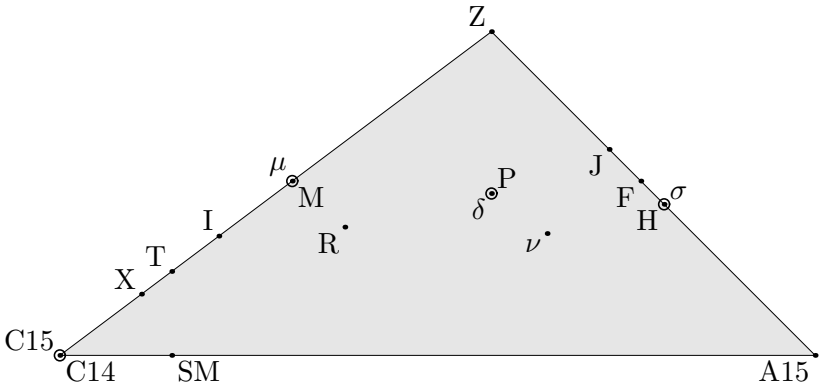


Figure 5. Every known TCP structure, when described by its numbers of 12-, 14-, 15-, and 16-sided cells, is a convex combination of the three basic structures A15, Z, and C15. Here the horizontal axis plots the average number of faces per cell (ranging from $13\frac{1}{3}$ to $13\frac{1}{2}$) and the vertical axis plots the fraction of cells which are 15-hedra (ranging from 0 to $\frac{2}{7}$). (Not all known structures are labeled in this picture.) Sometimes distinct structures appear at the same point in this triangle, but they need not then have the same properties.

Weaire-Phelan foam obtained there seems optimal among all TCP foams [KKPS]. This gives some evidence that this Weaire-Phelan foam may be the optimal solution to Kelvin's problem.

However, many of the TCP foams, like C15, T, and SM, have a cost significantly greater than Kelvin's. The fact that the Kelvin foam (with no pentagons) has such low cost means we must reëxamine our hypothesis that good foams need pentagons. In fact, we can find foams based on Voronoi cells for other crystal structures, like that of γ-brass, which do reasonably well, despite having even triangles among their faces. Thus it is hard to even guess where else to look for potential competitors for the optimal equal-volume foam, and we see little hope for any rigorous solution to Kelvin's problem; even the analogous problem in the plane is still open.

The fact that the Kelvin foam is not optimal suggests several related open problems worthy of consideration [SM]. It is interesting to note that the Weaire-Phelan foam does not have *equal pressures* in its cells, while the Kelvin foam does. (There has been repeated confusion in the literature between the equal-pressure and equal-volume conditions.) In fact, it seems that no foam in the A15 pattern (even allowing differing volumes) can have equal pressures.

In 1986, Kusner derived some necessary conditions for equal-pressure foams, such as a lower bound of $2 + 2\pi/\big(3\arccos(1/3) - \pi\big) > 13.39733$ on the average number of faces for a cell in the foam [Kus]. Choe proved that every compact three-manifold has a least-boundary-area fundamental domain [Cho]; the *Choe cells* for Euclidean manifolds all give equal-pressure, equal-volume foams in space. In fact, we know of no other equal-pressure foams. Perhaps these are the only combinatorial types of cells which can occur in such a foam. Presumably, for instance, no TCP pattern could yield an equal-pressure foam; many are already ruled out by the lower

bound above. We conjecture that the Kelvin foam is the Choe cell for the `bcc` torus, and is the best foam which has equal pressures as well as equal volumes.

References

[Alm] Fred Almgren. Computing soap films and crystals. In *Computing Optimal Geometries*, Selected Lectures in Mathematics, pages 3–5 plus video. Amer. Math. Soc., 1991.

[AKS] Fred Almgren, Rob Kusner, and John M. Sullivan. A comparison of the Kelvin and Weaire-Phelan foams. In preparation.

[ACI] Sigurd Angenent, David Chopp, and Tom Ilmanen. Nonuniqueness of mean curvature flow in $\mathbb{R}^3$. *Comm. Part. Diff. Eq.* To appear.

[Bra] Kenneth A. Brakke. The Surface Evolver. *Exper. Math.* **1**(1992), 141–165.

[Cho] Jaigyoung Choe. On the existence and regularity of fundamental domains with least boundary area. *J. Diff. Geom.* **29**(1989), 623–663.

[Cox] H. S. M. Coxeter. Close-packing and froth. *Ill. J. Math.* **2**(1958), 746–758.

[FK] F. C. Frank and J. S. Kasper. Complex alloy structures regarded as sphere packings. I. Definitions and basic principles. *Acta Crystallographica* **11**(1958), 184–190.

[Kel] Sir William Thomson (Lord Kelvin). On the division of space with minimum partitional area. *Acta Math.* **11**(1887), 121–134.

[KKPS] Andrew M. Kraynik, Rob Kusner, Robert Phelan, and John M. Sullivan. TCP structures as equal-volume foams. In preparation.

[Kus] Rob Kusner. The number of faces in a minimal foam. *Proc. R. Soc. Lond.* **439**(1992), 683–686.

[OBS] Atsuyuki Okabe, Barry Boots, and Kokichi Sugihara. *Spatial Tessellations: Concepts and Applications of Voronoi Diagrams.* Wiley & Sons, 1992.

[Pla] J. Plateau. *Statique Expérimentale et Théorique des Liquides Soumis aux Seules Forces Moléculaires.* Gauthier-villars, Paris, 1873.

[Riv] N. Rivier. Kelvin's conjecture on minimal froths and the counter-example of Weaire and Phelan. *Europhys. Lett.* **7**(1994), 523–528.

[Sen] Marjorie Senechal. *Crystalline Symmetries.* Adam Hilger, 1990.

[Sul] John M. Sullivan. The `vcs` software for computing voronoi diagrams. Available by email from `sullivan@@geom.umn.edu`.

[SM] John M. Sullivan and Frank Morgan (Editors). Open problems in soap bubble geometry: Posed at the Burlington Mathfest in August 1995. Preprint.

[Tay] Jean E. Taylor. The structure of singularities in soap-bubble-like and soap-film-like minimal surfaces. *Ann. of Math.* **103**(1976), 489–539.

[WP] Denis Weaire and Robert Phelan. A counter-example to Kelvin's conjecture on minimal surfaces. *Phil. Mag. Lett.* **69**(1994), 107–110.

[Wil] Robert E. Williams. Space filling polyhedron: Its relation to aggregates of soap bubbles, plant cells, and metal crystallites. *Science* **161**(July 1968), 276–277.