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A counter-example to Kelvin's conjecture on minimal surfaces

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ABSTRACT

Kelvin's conjecture, that a b.c.c. arrangement of his minimal tetrakaidecahedron divides space into equal cells of minimum surface area, has stood for over one hundred years. We have found a counter-example, in the form of a structure analogous to that of some clathrate compounds and also related to the β-tungsten structure. Its surface area is approximately 0·3% less than that of Kelvin's structure.

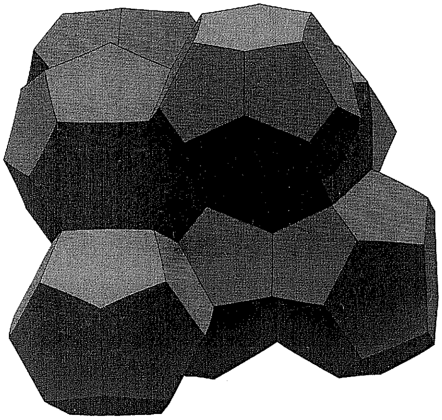
In 1887 the *Philosophical Magazine* published Kelvin's classic analysis of the following problem (Thomson 1887). What space-filling arrangement of cells of equal volume has minimum surface area? This arises naturally in the theory of foams, when the liquid content is small. It has an obvious solution in two dimensions, but not in three.

Kelvin was able to draw on the rules of Plateau (1873) for equilibrium structures of this kind. The surfaces which bound the cells must meet at 120° and the lines which are formed by their intersections must meet at $\cos^{-1}(-1/3)$, the tetrahedral angle. He proposed the body-centred-cubic (b.c.c.) structure as a likely candidate for the optimal arrangement. What is now familiar as the Wigner–Seitz (or Voronoi) cell of the b.c.c. structure is an orthic tetrakaidecadedron constructed from six square faces and eight hexagons. Kelvin showed how a slight distortion of the hexagonal faces was sufficient to satisfy Plateau's rules. He remarked that 'no shading could show satisfactorily the delicate curvature of the hexagonal faces'. Figure 1 illustrates this structure. The curvature reduces the surface area of the cell by about 0·2% (Princen and Levinson 1987).

That this should be the optimal solution is an appealing conjecture, implicit rather than directly stated in Kelvin's original papers. It is rather like the proposition that the density of face-centred-cubic (f.c.c.) is the maximum achievable for equal spheres, but it rests on even less firm ground. The question has often been raised, as to whether Kelvin's choice can be bettered. For example, the discussions of Williams (1968), Ross (1978) and Princen and Levinson (1987) all make interesting contributions, but no-one has hitherto succeeded in proving or disproving the conjecture. Particularly entertaining is the review by the botanist Matzke (1946) of various attempts to realize or observe the Kelvin structure in real systems. As for the mathematicians, they have generally maintained an open mind, but no less an authority than Weyl (1952) gave it as his opinion that is was unlikely that Kelvin's construction could be improved upon.

Recently Weaire (1994) has offered some speculation on a somewhat wider issue, that of the optimal structures of foams of finite liquid content (wet foam). In continuation of that line of thought we have begun calculations of surface energies of rival structures for dry foam, particularly the clathrate structures suggested by Weaire

Fig. 2



Unit cell of the space-filling structure reported here, with surface area minimized. It consists of six 14-sided polyhedra and two 12-sided polyhedra, as described in the text.

Isoperimetric quotient (figure of merit for area minimization) of various structures. An asterisk indicates non-space-filling cells.

Structure (lattice)	Isoperimetric quotient
Sphere*	1·000
Structure presented here (simple cubic lattice, eight cells)	0·764
Kelvin tetrakaidecahedron (b.c.c.)	0·757
Pentagonal dodecahedron*	0·7547
Orthic tetrakaidecahedron (b.c.c.)	0·7534
Rhombic dodecahedron (f.c.c.)	0·7405
Cube (s.c.)	0·5236

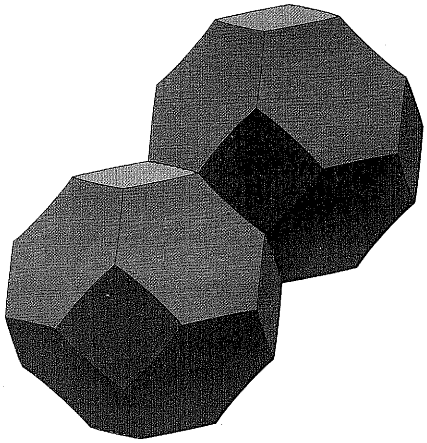
columns, the cells in each column being joined by their hexagonal faces. The pentagonal dodecahedra lie between them on a b.c.c. lattice. The overall lattice periodicity is simple cubic.

Note that the cell faces of this structure are irregular. Only the hexagonal faces remain planar (since they lie in symmetry planes of the structure).

There is another, and for some purposes simpler, way of describing the structure. The cell centres are the atomic positions of the β-W structure illustrated in fig. 3. This is one of the Frank–Kasper phases (see, for example, Pearson 1972). N. Rivier (private communication, 1993) has suggested that these should be of relevance to foam structures.

Of course, the structure discussed here can only be accorded the same provisional status as that previously enjoyed by Kelvin's, and it remains to be seen for how long it will hold the championship. In particular we have yet to check the other simple clathrate structure composed of pentagonal and hexagonal faces which arises in crystallography (Weaire 1994), as it has a much larger unit cell. It will be possible in due course to make exhaustive computer searches, but the intuition which suggested the structure here presented tends to the view that it will be difficult to surpass.

Fig. 1



Kelvin structure, constructed using the Surface Evolver package of K. Brakke (1992).

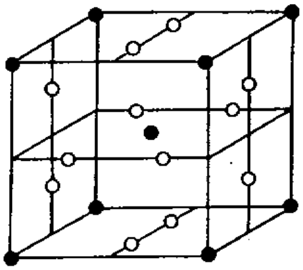
(1994) as a natural choice for intermediate values of liquid content. Our first result has immediate and largely unexpected implications. It overthrows Kelvin's conjecture by providing a counter-example which has a significantly lower surface energy.

The structure in question is derived from the periodic cubic clathrate structure of Na_8Si_{46} described by Kasper, Hagenmuller, Pouchard and Cros (1965). In this context, the cell vertices are tetrahedrally bonded Si atoms. These are entirely arranged in closed cages which enclose guest Na atoms, and can therefore be used to define a cellular structure. In adapting this simple clathrate to our purposes, we began with flat-sided polyhedral cells having the same topology. These were generated by a Voronoi construction using the Na positions as centres. The plane polyhedral cells generated by this initial construction do not have equal volumes. To equalize the volumes and produce the minimal structure we have used the 'Surface Evolver' package of Brakke (1992). This program minimizes surface area, subject to the constraint of fixed cell volumes, for successively finer tesselations of the original cell faces. In this way the curvature of the minimal surface can be progressively approximated with increasing accuracy. In the present case, the topology of the cellular structure is undisturbed by this relaxation.

Figure 2 shows one unit cell of the resulting structure. The table compares its surface energy with that of the Kelvin structure and some others. For consistency with some previous discussions we shall use as a figure of merit the so-called isoperimetric quotient defined by $36\pi V^2/A^3$. Here A is to be taken as the *average* cell surface area and V the cell volume. We see that the new structure has a surface energy which is approximately 0·3% less than that of Kelvin's solution, a remarkably large margin of superiority in this context.

Having established this result, we may rationalize it as follows. It has been repeatedly remarked that the ideal number of faces for a space-filling cell is close to fourteen: various geometrical/topological arguments point to this (Weaire and Rivier 1984). The 14-sided cell of least surface energy would appear to be that which consists of 12 pentagonal and two hexagonal faces. The clathrate structure which we have used consists mainly of such cells, with an admixture of one-third as many pentagonal dodecahedra. The 14-hedra are arranged in three mutually perpendicular, interlocking

Fig. 3



The β-W structure, in which the atomic positions correspond to the cell centres of the structure depicted in fig. 2

To many the assertion that Kelvin's elegant and simple solution is not optimal will come as a surprise, and the subject, together with its experimental counterpart in the observation of foams and emulsions, is thereby rendered even more intriguing. Our own experimental observations will be presented in a further paper (Weaire and Phelan 1994).

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