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A cubic Archimedean screw

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The Archimedean screw is a partition of space (more precisely, of a cylinder) into two congruent halves by a minimal surface (the helicoid). Fundamental to its function as a means of raising water are its handedness and an equivalence between continuous rotations and translations. Here a cubic crystalline structure is described that shares these properties. It consists of three infinite periodic minimal surfaces, each bounded by an infinite set of lines in $\langle 111 \rangle$ orientations arranged in a BCC lattice. The surfaces partition space into three congruent regions and meet at each bounding line forming 120° angles. Although screw-like rotation of the surfaces about the bounding lines is not an isometry, numerical calculations show that the surface area changes by only small fractions of a percent.

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1. Introduction

A number of amphiphile–water systems are known where the equilibrium structure changes from 'bicontinuous', a partition of space into two regions by a smooth surface, into a partition into hexagonal prisms, as the concentration is varied (for a survey of experimental results, see *J. Phys. Colloq.* **51** C7 (1990)). As a simple model, one supposes the surfaces which form the partition to be minimal and, as in the case of the hexagons, to form 120° angles whenever three surfaces meet along a curve. A geometrical parameter that distinguishes the two structures is the dimensionless boundary line density

$$l = \frac{LV}{A^2}, \tag{1.1}$$

where L and A are the total line length and surface area in a system of volume V. In the bicontinuous phase $l = 0$ while in the hexagonal phase $l = \sqrt{\tfrac{1}{3}}$. Are there equilibrium structures with intermediate values of l, possibly even sharing the cubic symmetry of the $l = 0$ structure?

2. Symmetry

As possible candidate structures one might first consider structures where the boundary curves, as in the hexagonal phase, are infinite lines. To ensure equilibrium at these lines it is also natural to satisfy the 120° angle constraint by symmetry. In a cubic structure this would mean that lines are oriented along each of the four $\langle 111 \rangle$ axes. Finally, the requirement that the lines avoid one another leads to the O^{8-} rod packing, well known in the study of blue phases (Meiboom *et al.* 1983). The structure

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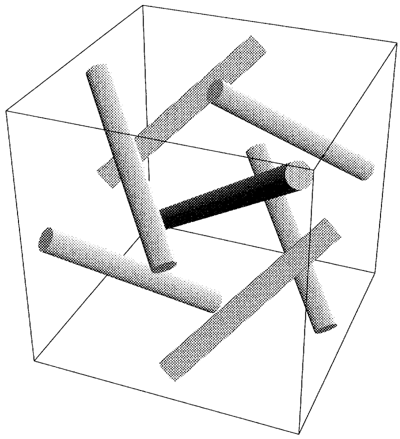

Figure 1. Rod packing associated with the cubic Archimedean screw. Three minimal surfaces meet at each rod forming 120° angles.

formed by the lines (figure 1) will then have space group $Ia\bar{3}d$. In the discussion and results presented below, we parametrize the lines as

$$\left.\begin{array}{cc}(0,0,0)+t(1,1,1), & (1,0,\tfrac{1}{2})+t(-1,1,1),\\ (\tfrac{1}{2},1,0)+t(1,-1,1), & (0,\tfrac{1}{2},1)+t\,(1,1,-1),\end{array}\right\} \tag{2.1}$$

where t is a real number. The Bravais lattice of the structure is BCC with the cubic lattice parameter $a=1$.

The three surfaces in our structure are conveniently described using a complex order parameter $\Psi(x,y,z)$. Boundary lines correspond to $\Psi=0$, while the surfaces themselves are defined by arg $\Psi=(\frac{2}{3}\pi)j$ with $j=0,\ \pm 1$. To formulate the symmetries of Ψ, we introduce the following space group generators:

$$r_3:(x,y,z)\rightarrow(y,z,x), \tag{2.2}$$

$$i:(x,y,z)\rightarrow(-x,-y,-z), \tag{2.3}$$

$$r_2:(x,y,z)\rightarrow(y-\tfrac{1}{4},x+\tfrac{1}{4},-z+\tfrac{1}{4}), \tag{2.4}$$

$$r_4:(x,y,z)\rightarrow(y+\tfrac{1}{4},-x+\tfrac{1}{4},z-\tfrac{1}{4}). \tag{2.5}$$

The set of boundary lines is invariant with respect to these transformations. Along the (111) axis the 120° angle relationship among the three surfaces is satisfied if we require

$$r_3(\Psi)=\omega\Psi, \tag{2.6}$$

where $\omega=\exp(\mathrm{i}\frac{2}{3}\pi)$. In fact, *six* surfaces would meet along (111) with 60° dihedral angles if Ψ were invariant with respect to inversion. We therefore insist that

$$\mathrm{i}(\Psi)=-\Psi. \tag{2.7}$$

This eliminates inversion as a symmetry and reduces the space group to $I4_132$.

By means of symmetry projection an expression for Ψ can be written that satisfies (2.6) and (2.7) and has specific symmetry properties with respect to the other generators, r_2 and r_4:

$$\Psi_\tau=\tfrac{1}{48}(1+\omega^2r_3+\omega r_3^2)(1-\mathrm{i})(1+r_2)(1+r_4+r_4^2+r_4^3)\mathrm{e}^{\mathrm{i}\tau}\rho(x,y,z). \tag{2.8}$$

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Here τ is a real parameter and ρ is an arbitrary real function belonging to the BCC Bravais class. Using the relations $r_2r_3 = r_3^2r_4$, $r_4r_3 = r_3^2r_4^3$, $r_4r_3^2 = r_3r_2$, $r_2r_4 = r_4^3r_2$, and the fact that i commutes with all the other generators, it is easily verified that

$$r_2(\Psi_\tau) = r_4(\Psi_\tau) = \exp(2\mathrm{i}\tau)\,\Psi_\tau^*. \tag{2.9}$$

We see that (2.9) preserves the sets $\arg \Psi_\tau = (\frac{2}{3}\pi)j$, $j = 0, \pm 1$ for $\tau = 0 \pmod{\frac{1}{3}\pi}$ and that r_2 and r_4 are not symmetries for other values of τ. On the other hand, since $r_4^2(\Psi_\tau) = \Psi_\tau$, we always have the smaller point group, T, or cubic space group $I2_13$. We have introduced τ, not because we believe the equilibrium (minimum area) structure has a lower symmetry, but because it provides a means of describing a screw-like deformation of the structure (see later). We note that a separate phase parameter is associated with each independent function ρ that is not annihilated by the projection operator in (2.8).

3. Fourier representation

In representing the familiar cubic minimal surfaces as level sets of periodic functions, experience has shown that the lowest-order Fourier modes (consistent with the space group) give not only the correct topology but also a reasonably accurate approximation of the true shape (von Schnering & Nesper 1987). When we try this with the present problem we find one (linearly independent) function at lowest order:

$$\rho(x, y, z) = \sin(2\pi x)\cos(2\pi y). \tag{3.1}$$

The next non-vanishing modes have a considerably larger wavevector, $2\pi(211)$. By varying the 'twist-angle' τ associated with the lowest mode (3.1), we obtain a continuous family of deformations (figure 2) that generates a cyclic permutation of the three surfaces after τ has changed by $\frac{2}{3}\pi$. The variation of the area, $A(\tau)$, with τ gives some indication of how closely the twisting of the surfaces can mimic the true screw isometry of the helicoid. In investigating $A(\tau)$ we may restrict ourselves to the range $0 \leqslant \tau < \frac{1}{6}\pi$ since $A(\tau) = A(\tau + \frac{1}{3}\pi)$ and $A(\tau) = A(-\tau)$. The former follows from $\Psi_{\tau+\pi/3} = \mathrm{i}r_3^2\Psi_\tau$ and the latter from $\Psi_{-\tau} = r_2\Psi_\tau^*$.

4. Numerical method

An easily implemented, though highly inefficient, method of computing the surface area of an implicitly defined surface, $f(x, y, z) = 0$, is based on the formula

$$A = \int |\nabla f|\delta(f)\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z, \tag{4.1}$$

with the delta function replaced by

$$\delta(f) \approx \frac{1}{\sqrt{\pi}\epsilon}\exp[-(f/\epsilon)^2]. \tag{4.2}$$

By evaluating (4.1) on a regular grid and taking a sequence of decreasing values of ϵ, the areas given in table 1 are obtained. A very fine grid (spacing $\frac{1}{400}$) and small epsilon (0.05) is needed to resolve the minute area variation with τ. As expected, the least area corresponds to the highest point group symmetry, $\tau = 0$. More interesting and also the basis of the analogy with the Archimedean screw, is the fact that these

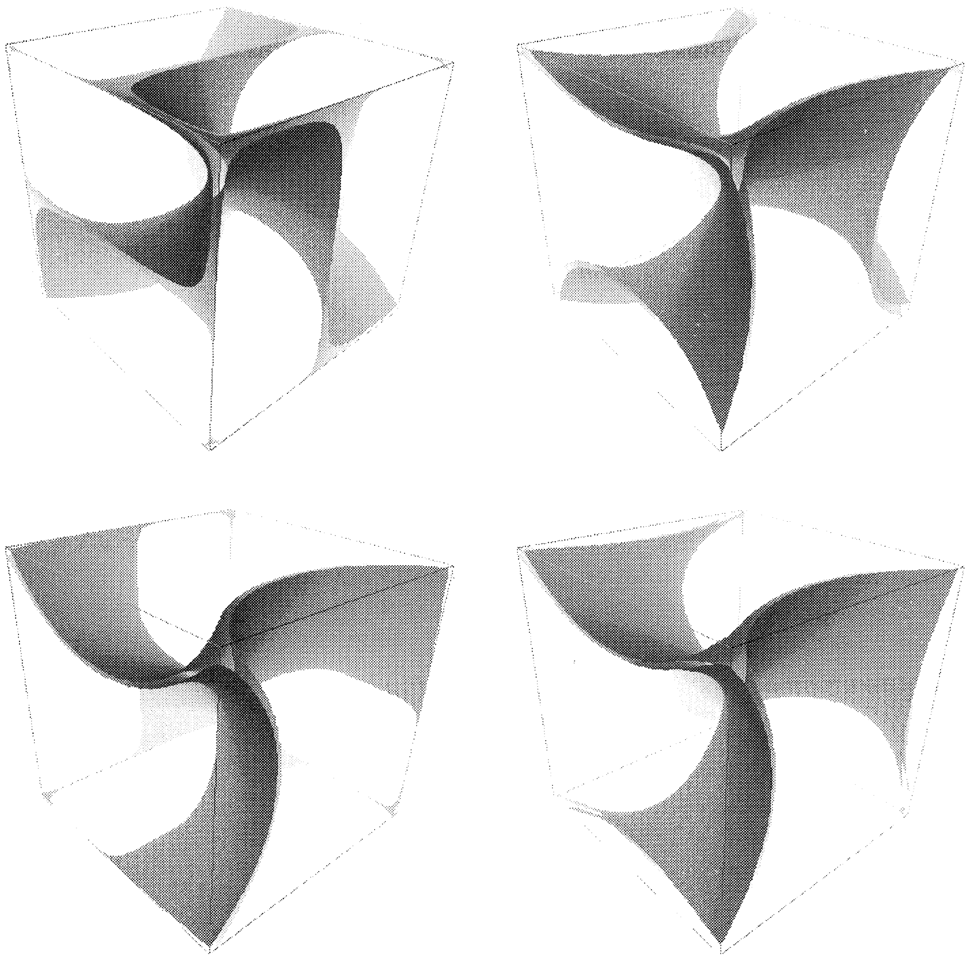

Figure 2. Deformations of the cubic Archimedean screw for twist angles $\tau = 0°$, $20°$, $40°$ and $60°$, clockwise, beginning with the upper left corner. Shown is one octant of the conventional cubic cell. The three surfaces correspond to the level set $|\Psi|^3 - \mathrm{Re}(\Psi^3) = \delta$ for small positive δ. In the limit $\delta \to 0$, the surfaces coalesce pairwise, with pairs meeting at $120°$ angles along the body diagonal. As explained in the text, the deformation $\tau = 60°$ corresponds to the inversion of $\tau = 0°$.

area variations are indeed so small. Relaxation of the surface, say by including higher-order Fourier modes, should not alter the conclusion that there exist permutation-generating deformations that increase the area by only a fraction of a percent. Using $A \approx 2.34$ we obtain $l \approx 0.316$ for the dimensionless line density (1.1).

5. Properties

Handedness does not imply that the three surfaces wind helix-like about the boundary lines. For the lowest-order Fourier representation (3.1) of Ψ, the winding angle ϕ of one surface about the line $t(1,1,1)$ is given by the formula

$$\phi = \tau + \arg[\cos^2(2\pi t) - \omega^2 \sin^2(2\pi t)]. \tag{5.1}$$

Table 1. *Total area, $A(\tau)$, per primitive BCC cell as a function of the twist angle τ*

τ	0°	5°	10°	15°	20°	25°	30°
$A(\tau)$	2.3399	2.3402	2.3410	2.3422	2.3434	2.3442	2.3443

This shows that in fact ϕ only oscillates between two extremes—the angular range being 60° for our approximate representation. Handedness, nevertheless, manifests itself in true screw-like fashion if we imagine an experiment where laser light is reflected from the surface as the twist angle τ is rotated. Suppose the laser beam is directed at the structure along the z-axis and a single source of back-scattering is followed. In particular, it can be easily verified (again, using the lowest order Fourier representation) that the point $(\frac{1}{2}, \frac{1}{4}, z(\tau))$, where

$$\tan\left[2\pi z(\tau)\right] = \frac{\sin(\tau - \frac{2}{3}\pi)}{\sin(\tau + \frac{2}{3}\pi)}, \tag{5.2}$$

lies on the surface $\arg \Psi = 0$ and the surface normal is parallel to the z-axis. If $\frac{2}{3}\pi$ in (5.2) were replaced by $\frac{3}{4}\pi$, we would have $z(\tau) = -\tau/(2\pi) - \frac{1}{8}$. In fact, the monotonic decrease in the height $z(\tau)$ of the point of reflection with the twist parameter τ is accompanied by undulations.

6. Conclusions

The cubic Archimedean screw fills a gap in the universe of structures built from minimal surfaces or pieces of minimal surfaces joined in soap-froth fashion. The known cubic structures either consist of a single surface or are Voronoi-like froths where both the minimal surface patches and the boundary curves are finite. The only known, and nevertheless important, example of a structure with infinite boundary curves is the honeycomb. The cubic Archimedean screw can therefore be viewed as an example of a 'cubic honeycomb'. It is interesting that handedness is a property of what appears to be the simplest example of a cubic honeycomb.

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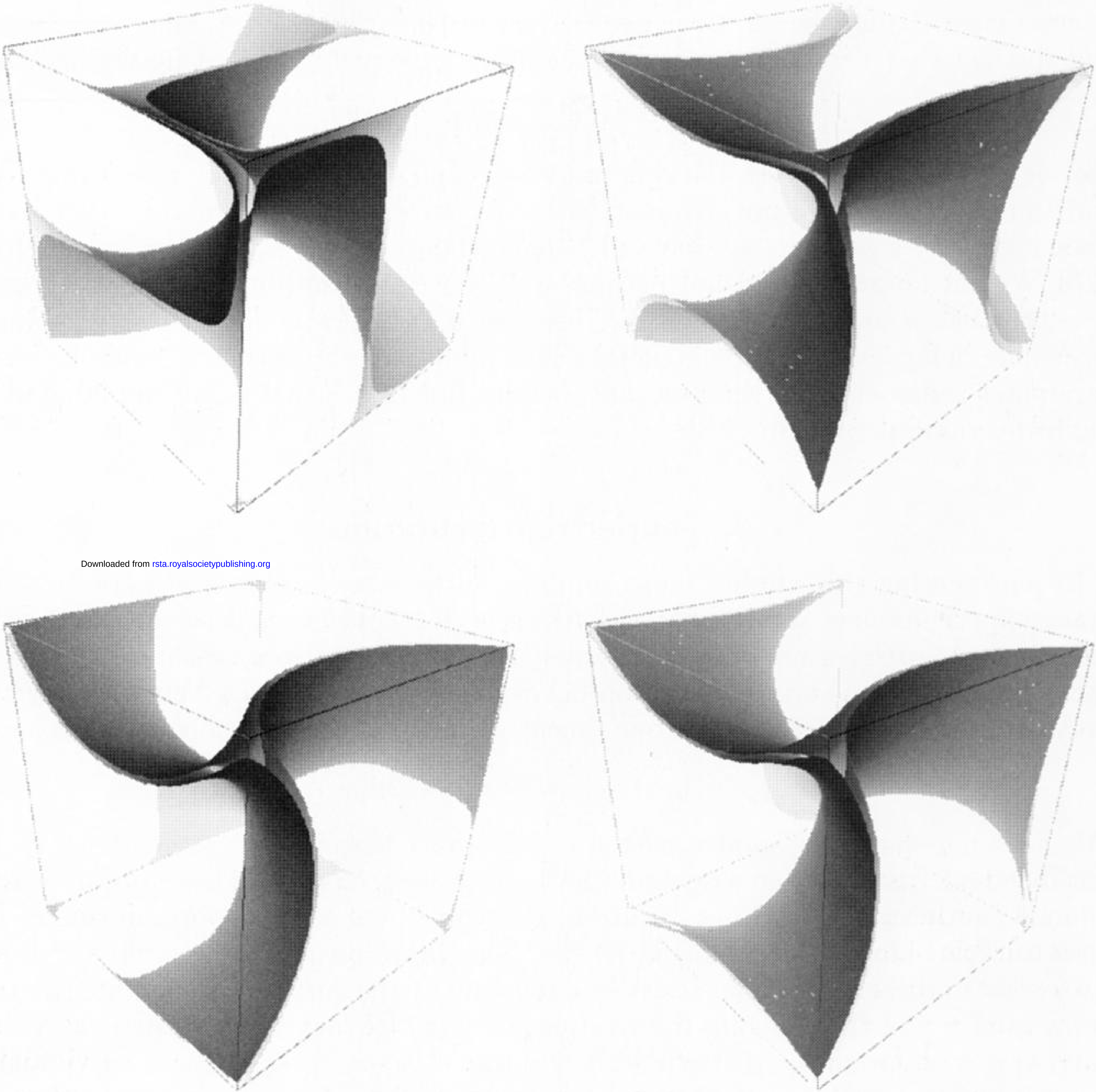

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