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Minimal surfaces and multifunctionality

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Triply periodic minimal surfaces are objects of great interest to physical scientists, biologists and mathematicians. It has recently been shown that triply periodic two-phase bicontinuous composites with interfaces that are the Schwartz primitive (P) and diamond (D) minimal surfaces are not only geometrically extremal but extremal for simultaneous transport of heat and electricity. More importantly, here we further establish the multifunctionality of such two-phase systems by showing that they are also extremal when a competition is set up between the effective bulk modulus and the electrical (or thermal) conductivity of the composite. The implications of our findings for materials science and biology, which provides the ultimate multifunctional materials, are discussed.

Keywords: minimal surfaces; multifunctionality; composites; elastic moduli; conductivity; optimization

1. Introduction

A minimal surface, such as a soap film, is one that is locally area minimizing. Surface tension minimizes the energy of the film, which is proportional to its surface area. Minimal surfaces necessarily have zero mean curvature, i.e. the sum of the principal curvatures at each point on the surface is zero. Particularly fascinating are minimal surfaces that are triply periodic because they arise in a variety of systems, including block copolymers (Olmstead & Milner 1998), nanocomposites (Yunfeng *et al*. 2001), micellar materials (Ziherl & Kamien 2000), lipid bilayers (Gelbart *et al*. 1994), and other biological formations (National Research Council 1996). These two-phase composites are bicontinuous in the sense that the surface (two-phase interface) divides space into two disjoint but intertwining phases that are simultaneously continuous. This topological feature of bicontinuity is rare in two dimensions and is therefore virtually unique to three dimensions (Torquato 2002).

It has recently come to light that triply periodic two-phase bicontinuous composites with interfaces that are the Schwartz primitive (P) and diamond (D) minimal surfaces (see figure 1) are not only geometrically extremal but extremal for simultaneous transport of heat and electricity (Torquato *et al*. 2002, 2003). More specifically, these are the optimal structures when a weighted sum of the effective thermal and electrical conductivities is maximized for the case in which phase 1 is a good thermal conductor but a poor electrical conductor and phase 2 is a poor thermal conductor but a good electrical conductor. The demand that this sum is maximized sets

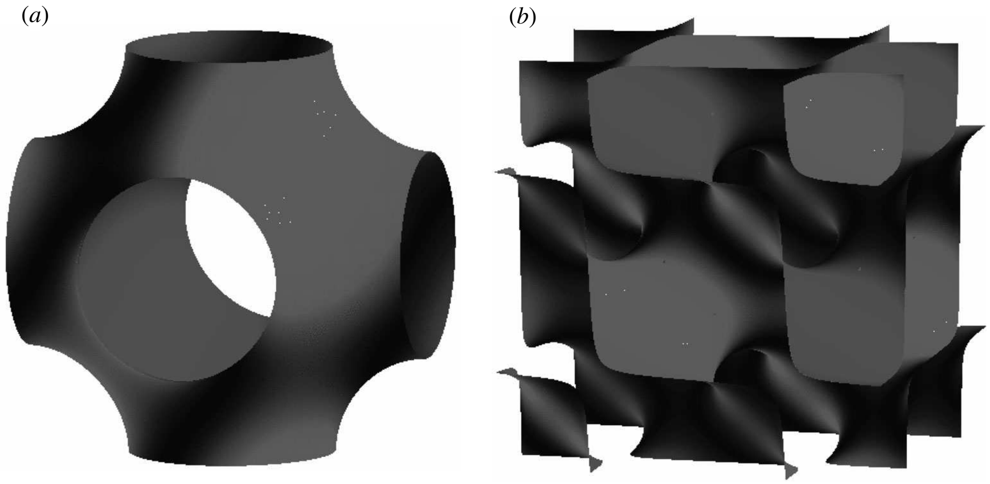

Figure 1. Unit cells of two different minimal surfaces with a resolution of $64 \times 64 \times 64$. (a) Schwartz simple cubic surface. (b) Schwartz diamond surface.

up a *competition* between the two effective transport properties, and this demand is met by the Schwartz P and D structures. By mathematical analogy, the optimality of these bicontinuous composites applies to any pair of the following scalar effective properties: electrical conductivity, thermal conductivity, dielectric constant, magnetic permeability and diffusion coefficient.

The topological property of bicontinuity of these structures suggests that they would be mechanically stiff even if one of the phases was a compliant solid or a liquid, provided that the other phase is a relatively stiff material. The demonstration that the Schwartz P and D structures also have desirable mechanical properties is in some sense more important than showing that they have extremal transport properties, since one can find single-phase materials that are good electrical and thermal conductors. Indeed, here we further establish the multifunctionality of such two-phase systems by demonstrating that they are extremal when a competition is set up between the bulk modulus and the electrical (or thermal) conductivity of the composite. The ultimate multifunctional materials are provided by nature; virtually all biological material systems are composites that typically are endowed with a superior set of properties. Biological systems must be able to perform a variety of functions well, i.e. roughly speaking, biological materials are 'optimized' for multifunctional purposes. The intriguing implications of our findings for materials science and biology are discussed after we prove the aforementioned claims employing cross-property bounds.

2. Cross-property bounds

Consider a two-phase composite material in which phase i has electrical conductivity σ_i, bulk modulus K_i, shear modulus G_i, and volume fraction ϕ_i, where $i = 1$ or 2. We denote by σ_e and K_e the effective conductivity and effective bulk modulus of the composite, respectively. For simplicity, we will assume that $\phi_1 = \phi_2 = \frac{1}{2}$ and we examine 'ill-ordered' cases of a two-phase composite material in which phase 1 is more conducting but less stiff than phase 2, i.e.

$$\frac{\sigma_1}{\sigma_2} > 1, \qquad \frac{K_1}{K_2} < 1, \qquad \frac{G_1}{G_2} < 1. \tag{2.1}$$

As we will explain below, this situation is motivated by examples that arise in biology and materials science. We now ask what are the two-phase composite structures that maximize a weighted sum of the dimensionless effective bulk modulus K_e/K_1 and effective electrical conductivity σ_e/σ_2? Thus, we set up a competition between a mechanical property and a transport property. It is hypothesized that the optimal solutions are the same triply periodic minimal surfaces that maximize a weighted sum of the thermal and electrical conductivities (Torquato *et al*. 2002, 2003).

To prove our assertion, we apply *cross-property* bounds for two-phase composites that rigorously link the effective bulk modulus to the effective electrical conductivity given the phase elastic moduli and conductivities (Gibiansky & Torquato 1996). The bulk modulus measures the elastic resistance to hydrostatic compression or expansion of the material. In general, cross-property bounds provide a means of ascertaining the possible range of values that different effective properties can possess, i.e. the allowable region in multidimensional property space, and thus have important implications for the design of *multifunctional* composites (Torquato 2002). Why should cross-property relations even exist in the case of composites? We know that such correlations do not generally exist for single-phase materials. However, in the case of composites, the underlying microstructure provides the link that enables one to generally relate one effective property to a different effective property of the same composite. The reason is that an effective property provides a certain average measure of the microstructure, and thus it is not surprising that cross-property relations exist (Torquato 2002).

Using the translation method, Gibiansky & Torquato (1996) derived the sharpest known cross-property bounds linking the effective conductivity σ_e to the effective bulk modulus K_e for three-dimensional two-phase composites of all possible microstructures at a prescribed or arbitrary volume fraction. The translation bounds are described by hyperbolas in the (σ_e, K_e)-plane with asymptotes that are parallel to the axes $\sigma_e = 0$ and $K_e = 0$. Every hyperbola in the plane can be defined by three points that it passes through. We denote by $\mathrm{Hyp}[(x_1, y_1), (x_2, y_2), (x_3, y_3)]$ the segment of the hyperbola that joins the points (x_1, y_1), (x_2, y_2), and when extended passes through the point (x_3, y_3). It may be parametrically described in the (x_e, y_e)-plane as

$$x_e = \langle x \rangle_\alpha - \frac{\alpha(1-\alpha)(x_1 - x_2)^2}{x_1(1-\alpha) + x_2\alpha - x_3}, \qquad y_e = \langle y \rangle_\alpha - \frac{\alpha(1-\alpha)(y_1 - y_2)^2}{y_1(1-\alpha) + y_2\alpha - y_3}, \tag{2.2}$$

where $\langle x \rangle = x_1\alpha + x_2(1-\alpha)$, $\langle y \rangle = y_1\alpha + y_2(1-\alpha)$ and $\alpha \in [0, 1]$. Before stating the translation bounds, we first introduce some notation. Denote by $F_a(y)$ the function

$$F_a(y) = a_1\phi_1 + a_2\phi_2 - \frac{\phi_1\phi_2(a_1 - a_2)^2}{a_1\phi_2 + a_2\phi_1 + y}. \tag{2.3}$$

Let σ_{1*}, σ_{2*}, $\sigma_{1\#}$, $\sigma_{2\#}$, K_{1*}, K_{2*}, σ_a, σ_h, K_a, K_h denote the expressions

$$\begin{aligned} \sigma_{1*} &= F_\sigma(2\sigma_1), \qquad \sigma_{2*} = F_\sigma(2\sigma_2), \qquad \sigma_{1\#} = F_\sigma(-2\sigma_1), \\ \sigma_{2\#} &= F_\sigma(-2\sigma_2), \qquad K_{1*} = F_K(4G_1/3), \qquad K_{2*} = F_K(4G_2/3), \\ \sigma_a &= \phi_1\sigma_1 + \phi_2\sigma_2 = F_\sigma(\infty), \qquad \sigma_h = \left(\frac{\phi_1}{\sigma_1} + \frac{\phi_2}{\sigma_2}\right)^{-1} = F_\sigma(0), \\ K_a &= \phi_1 K_1 + \phi_2 K_2 = F_K(\infty), \qquad K_h = \left(\frac{\phi_1}{K_1} + \frac{\phi_2}{K_2}\right)^{-1} = F_K(0). \end{aligned}$$

Cross-property bounds on the set of the pairs (σ_e, K_e) for any two-phase composite that is isotropic or possesses cubic symmetry at a fixed volume fraction $\phi_1 = 1 - \phi_2$ are defined by the segments of the following five hyperbolas in the (σ_e, K_e)-plane (Gibiansky & Torquato 1996):

$$\mathrm{Hyp}[(\sigma_{1*}, K_{1*}), (\sigma_{2*}, K_{2*}), (\sigma_1, K_1)], \quad \mathrm{Hyp}[(\sigma_{1*}, K_{1*}), (\sigma_{2*}, K_{2*}), (\sigma_2, K_2)], \tag{2.4}$$

$$\mathrm{Hyp}[(\sigma_{1*}, K_{1*}), (\sigma_{2*}, K_{2*}), (\sigma_{1\#}, K_h)], \quad \mathrm{Hyp}[(\sigma_{1*}, K_{1*}), (\sigma_{2*}, K_{2*}), (\sigma_{2\#}, K_h)], \tag{2.5}$$

$$\mathrm{Hyp}[(\sigma_{1*}, K_{1*}), (\sigma_{2*}, K_{2*}), (\sigma_a, K_a)]. \tag{2.6}$$

The outermost pair of these curves give us the desired bounds. In some cases, points along the bounds are known to be realizable by certain two-phase microstructures. In such instances, the bounds are optimal (best possible) given the volume fraction.

For the case of ill-ordered phases defined by relation (2.1), the cross-property lower bound and upper bound are given by the second hyperbola in (2.5) and the hyperbola in (2.6), respectively. The cross-property upper bound in particular provides the locus of points that maximizes the weighted sum $wK_e/K_1 + (1-w)\sigma_e/\sigma_2$ for a range $0 < w < 1$. For the special case $\phi_1 = \phi_2 = \frac{1}{2}$, the point on the upper bound (σ_e^U, K_e^U) corresponding to $\alpha = \frac{1}{2}$ can be expressed exactly by

$$\sigma_e^U = \frac{2\sigma_1\sigma_2 + (\sigma_1 + \sigma_2)^2}{3(\sigma_1 + \sigma_2)}, \qquad K_e^U = \frac{2[3K_1K_2 + (K_1 + K_2)(G_1 + G_2)]}{3(K_1 + K_2) + 4(G_1 + G_2)}. \tag{2.7}$$

This point on the upper bound is optimal because it is realizable by a special *bicontinuous multiscale* composite (Gibiansky & Torquato 1996): a polycrystal in which each grain is composed of a laminate consisting of alternating slabs of phases 1 and 2 such that the slab thicknesses are much smaller than the size of the grain and the grains are randomly oriented.

(*a*) *Optimality of Schwartz P and D structures*

It remains now to show that two-phase *single-scale* bicontinuous composites with Schwartz P and D interfaces also correspond to the optimal upper bound point (σ_e^U, K_e^U) defined by (2.7). To accomplish this, we use potential representations of the minimal surfaces to generate discretizations of these bicontinuous two-phase composites. We then used a finite-element code to calculate numerically the corresponding effective bulk moduli and conductivities for a wide range of phase conductivities and moduli that meet the 'ill-ordered' condition (2.1). Indeed, independent of the phase properties, we have found that the calculated pair of effective properties (within small

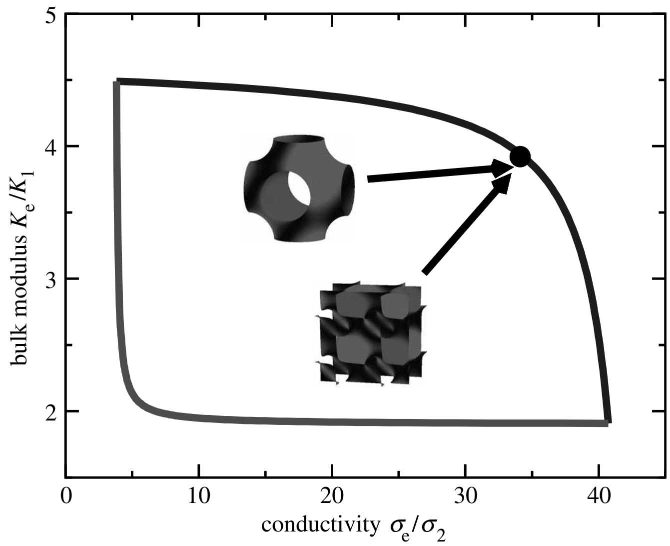

Figure 2. Cross-property bounds for the effective conductivity σ_e and effective bulk modulus K_e for ill-ordered phases in which $\sigma_1 = 100$, $\sigma_2 = 1$, $K_1 = 1$, $K_2 = 10$, $G_1 = 1$ and $G_2 = 100$. The simulation datum on the upper bound corresponds to the bicontinuous P and D Schwartz structures in which $\phi_1 = \phi_2 = \frac{1}{2}$.

numerical error) correspond to the optimal upper bound point (2.7). This result is not unexpected because it was shown that the aforementioned bicontinuous multi-scale composite and the Schwartz P and D surfaces realize an analogous point on the upper bound linking the effective electrical and thermal conductivities (Torquato *et al*. 2002, 2003). Figure 2 compares the numerical calculation with cross-property bounds for the particular case $\sigma_1 = 100$, $\sigma_2 = 1$, $K_1 = 1$, $K_2 = 10$, $G_1 = 1$ and $G_2 = 100$. Note that the shape of the upper bound in figure 2 in the extreme case of a conducting liquid ($\sigma_1 = 1$, $G_1 = 0$, $K_1 \neq 0$) and a non-conducting solid ($\sigma_1 = 0$, $G_2 \neq 0$, $K_2 \neq 0$) remains qualitatively the same.

It is noteworthy that if one breaks the symmetry of the problem by moving off the point (2.7) (corresponding to $\phi_1 = \phi_2 = \frac{1}{2}$ and/or $\alpha = \frac{1}{2}$), the optimal structure (if it exists) will still be bicontinuous within a neighbourhood of the point (2.7) but will not be a minimal surface. In future studies, it will be interesting to investigate whether such structures are bicontinuous structures with interfaces of constant mean curvature, which become minimal surfaces at the point $\phi_1 = \phi_2 = \frac{1}{2}$. Two-phase composites with interfaces of constant mean curvature are also objects of great interest (Anderson *et al*. 1990). Although four other points along the cross-property upper bound are known to be realizable (Gibiansky & Torquato 1996), it is not known whether all of the points along this curve are realizable.

3. Resistance to shear

An important practical question is to what extent can the Schwartz P and D bicontinuous structures withstand shear stresses? Since these structures have cubic elastic symmetry, they possess not only an effective bulk modulus K_e but two independent effective shear moduli. Thus, these composites cannot be expected to have optimal shear moduli, but it would be useful to know whether they are reasonably resistant to shear. To answer this question, we choose to study the two effective shear moduli G_{e} and ΔG_{e} defined by

$$G_{\mathrm{e}} \equiv \tfrac{1}{2}((C_{11})_{\mathrm{e}} - (C_{12})_{\mathrm{e}}), \qquad \Delta G_{\mathrm{e}} = G_{\mathrm{e}} - (C_{44})_{\mathrm{e}}, \tag{3.1}$$

where $(C_{11})_{\mathrm{e}}$, $(C_{12})_{\mathrm{e}}$ and $(C_{44})_{\mathrm{e}}$ are the components of the effective stiffness tensor for cubic elastic symmetry (Torquato 2002). Note that ΔG_{e} is a measure of elastic anisotropy, i.e. when the composite is elastically isotropic, $\Delta G_{\mathrm{e}} = 0$, and there is only one effective shear modulus, namely, G_{e}. We have computed G_{e} and ΔG_{e} using finite elements for all of the cases considered above and found that this pair of shear moduli are different for the Schwartz P and D structures.

We also compared these simulation data with rigorous upper and lower bounds given by

$$\frac{(2\Delta G_{\mathrm{e}} + 5G_1 - 5G_{\mathrm{e}})\phi_1}{(G_1 - G_{\mathrm{e}})(\Delta G_{\mathrm{e}} - G_{\mathrm{e}} + G_1)} = \frac{5}{G_2 - G_1} + \frac{6(K_1 + 2G_1)\phi_2}{G_1(3K_1 + 4G_1)}, \tag{3.2}$$

$$\frac{(2\Delta G_{\mathrm{e}} + 5G_2 - 5G_{\mathrm{e}})\phi_2}{(G_2 - G_{\mathrm{e}})(\Delta G_{\mathrm{e}} - G_{\mathrm{e}} + G_2)} = \frac{5}{G_1 - G_2} + \frac{6(K_2 + 2G_2)\phi_1}{G_2(3K_2 + 4G_2)}, \tag{3.3}$$

which apply when $G_2 \geqslant G_1$. In the $(G_{\mathrm{e}}, \Delta G_{\mathrm{e}})$-plane, relation (3.2) provides an upper bound on G_{e} for fixed ΔG_{e} (a lower bound on ΔG_{e} for fixed G_{e}) and relation (3.3) provides a lower bound on G_{e} for fixed ΔG_{e} (an upper bound on ΔG_{e} for fixed G_{e}). It is a simple matter to derive these bounds, which are valid for a two-phase composite with cubic elastic symmetry, from the general anisotropic bounds of Milton & Kohn (1988). Note that when $\Delta G_{\mathrm{e}} = 0$, these bounds reduce to the well-known Hashin–Shtrikman bounds for isotropic composites (Hashin & Shtrikman 1963). It is seen from figure 3 that the simulation data lie roughly between the upper and lower bounds for the case corresponding to figure 2. This is true even in the limit $G_1/G_2 \to 0$. Therefore, these bicontinuous composites are relatively resistant to shear as well.

4. Conclusions and discussion

The multifunctional character of triply periodic Schwartz P and D bicontinuous composites has been further revealed in this paper. Earlier it was shown that these bicontinuous structures are extremal when a competition is set up between any two pairs of the following effective properties: electrical conductivity, thermal conductivity, dielectric constant, magnetic permeability and diffusion coefficient (Torquato *et al.* 2002, 2003). More importantly, here we establish that they are also extremal when a competition is set up between the effective bulk modulus and any of the aforementioned 'transport' properties; for concreteness, we focused here on the electrical conductivity. Moreover, we have shown that Schwartz P and D structures are relatively stiff in shear. We expect that when one phase is a fluid, such a bicontinuous porous medium will have a reasonably large fluid permeability. How close such structures are to being extremal when the fluid permeability competes against other effective properties will be the subject of a future investigation.

We believe that our results have intriguing implications for the systematic design of novel multifunctional materials. The current trend to develop multifunctional materials has been further fuelled by progress in our ability to synthesize new materials

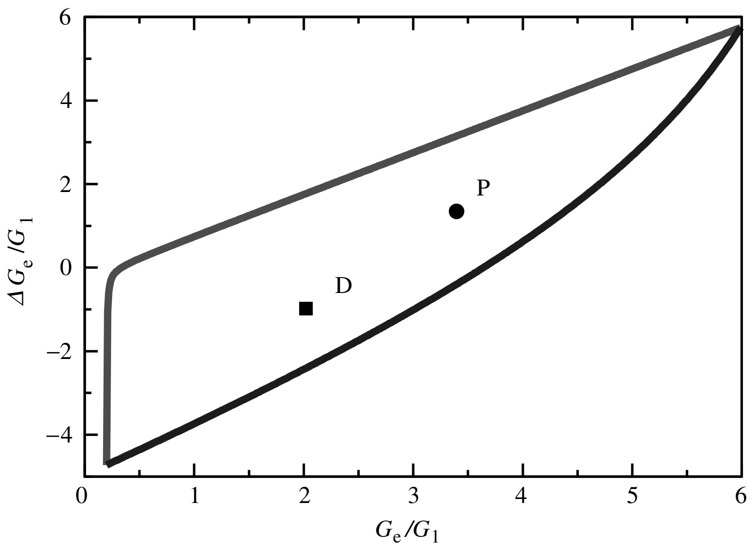

Figure 3. Bounds on the two effective shear moduli ΔG_e and G_e for ill-ordered phases in which $K_1 = 1$, $K_2 = 10$, $G_1 = 1$ and $G_2 = 100$. The simulation data correspond to the bicontinuous P and D Schwartz structures.

and to design and analyse materials via computer simulations. Desirable multifunctional requirements include component structures that have novel mechanical, thermal, electromagnetic, chemical and flow properties, and low weight. It is difficult to find single homogeneous materials that possess these multifunctional characteristics. Composite materials are ideally suited to achieve multifunctionality since the best features of different materials can be combined to form a new material that has a broad spectrum of desired properties. In this regard it is noteworthy that Schwartz P and D bicontinuous composites or porous media can presently be fabricated on a wide range of length-scales using self-assembly processing techniques (Olmstead & Milner 1998; Yunfeng *et al*. 2001) and therefore such multifunctional bicontinuous materials should find a host of applications. One could imagine combining the very high electrical conductivity of compliant conducting polymers with a non-conducting ceramic phase to provide overall stiffness. Depending on the application, the ceramic phase in this example could be replaced by a metallic phase with a high thermal conductivity in order to dissipate heat. When one phase is a liquid and the other phase is a stiff solid, triply periodic Schwartz P and D bicontinuous porous media can serve as mechanically stiff highly selective sieves for macromolecules and other particles moving in the liquid of sizes of the order of the well-defined pore sizes.

Finally, it is interesting to comment on the formation of triply periodic Schwartz P and D bicontinuous porous media that arise in biology; a case in point being cell membranes (National Research Council 1996). It would be fascinating to ascertain whether simple biological systems or subsystems are truly optimized in a rigorous mathematical sense. Species themselves are not optimized in such a sense. One reason for this is that species do not have to be globally optimized to survive and adapt to changes in their environments. Species simply have to be fit enough, not optimal. Moreover, to understand the evolution of species from an optimization point of view would require knowledge that is impossible to ascertain precisely today. For example, which functions did the organism have to perform well and at what times? Under what constraints did it evolve? The number of variables, conditions and constraints can be quite large.

Even though life itself is not optimized in a strict mathematical sense, it is possible that subsystems within an organism, such as cell membranes, are truly optimized. We have shown that the bicontinuous porous media that arise in cell membranes are extremal when a variety of different functions compete against one another. Although this does not prove that this subsystem was optimized by evolutionary processes, it is rather suggestive. Cell membranes have evolved to allow a variety of different transport processes to occur (e.g. diffusional and electrical) and they must also be stiff enough to act as a structure. It may prove fruitful to examine whether the optimization of competing functionalities in biological subsystems can explain their resulting structures.

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