Optimizing the bulk modulus of cellular networks

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Abstract

We present an alternative derivation of upper-bounds for the bulk modulus of both two-dimensional and three-dimensional cellular materials. For two-dimensional materials, we recover exactly the expression of the Hashin-Shtrikman (HS) upper-bound in the low-density limit, while for three-dimensional materials we even improve the HS bound. Furthermore, we establish necessary and sufficient conditions on the cellular structure for maximizing the bulk modulus, for a given solid volume fraction. These conditions are found to be exactly those under which the electrical (or thermal) conductivity of the material reaches its maximal value as well. These results provide a set of straightforward criteria allowing to address the design of optimized cellular materials, and shed light on recent studies of structures with both maximal bulk modulus and maximal conductivity. Finally, we discuss the compatibility of the criteria presented here with the geometrical constraints caused by minimization of surface energy in a real foam.

Cellular solids appear widely in nature and are manufactured on a large scale by man. Examples include wood, cancellous bone, cork, foams for insulation and packaging, or sandwich panels in aircraft. Material density, or solid volume fraction, ϕ, is a predominant parameter for the mechanical properties of cellular materials. Various theoretical studies on the mechanical properties of both two-dimensional (2D) and three-dimensional (3D) structures have been attempted [1]. Unfortunately, exact calculations can be achieved for cellular materials with simple geometry only [2], and numerical simulations [2][3] or semi-empirical models [4][5][6] are required in order to study the mechanical properties of more complex structures. However, expression of bounds on the effective moduli can be established. Perhaps the most famous bounds are those given by Z. Hashin and S. Shtrikman for isotropic heterogeneous media [7][8]. In particular, the Hashin-Shtrikman bounds for the effective bulk modulus in the low-density asymptotic limit ($\phi \ll 1$) read:

$$0 \leq \kappa^{(2D)} \leq \frac{E\phi}{4} \tag{1}$$

for 2D cellular structures [7][9], and:

$$0 \leq \kappa^{(3D)} \leq \frac{4E\phi}{9}\frac{G+3K}{4G+3K} \tag{2}$$

for 3D structures [8]. $\kappa^{(2D)}$ and $\kappa^{(3D)}$ are the actual bulk modulus respectively for 2D and 3D structures, and E, G, K are the Young modulus, shear modulus, and bulk modulus of the solid phase, respectively. These three elastic moduli are related by: $E = \frac{4KG}{K+G}$ for 2D bodies and by: $E = \frac{9KG}{3K+G}$ for 3D bodies.

The search for optimal structures maximizing some specific modulus (for a given value of solid volume fraction ϕ), is of evident practical importance. In a recent study, Torquato et al. [9][10] identified values of conductivity and elastic moduli of the two-dimensional square, hexagonal, kagomé and triangular cellular structures, and observed that the bulk modulus of these structures is equal to the HS upper-bound value. The authors did not attempt to explain this result, although they noticed that such structures under uniform compression deform without bend (affine compression). Are these structures the only structures with maximal bulk modulus ? And if they are not, can we provide criteria on the structure of "optimized" cellular materials ? More intriguingly, Torquato et al. noticed that these structures present maximal electrical (or thermal) conductivity as well. Is this feature caused by the particular symmetry of the studied strutures, or is there an underlying relation between the conductivity and the bulk modulus of cellular materials ? We shall answer to all these questions in the present study. Indeed, Durand & Weaire [11][12] already established necessary and sufficient conditions on the structure of cellular networks having maximal average conductivity. A quite similar approach is used in this paper to show that the very same conditions are also necessary and sufficient to maximize the bulk modulus of an open-cell material. There are some evident similarities between the constitutive laws (Ohm's law and Kirchhoff's laws) of electrical current in wires and those of the thin beam theory, but complexity is increased in the latter case, the scalar quantities I (the electrical current) and V (the electrical potential) being replaced by the vectorial quantities $\mathbf{F}$ (force acting on a beam) and $\mathbf{u}$ (the displacement field).

We consider first the case of a 2D cellular material. We suppose its solid volume fraction ϕ is sufficiently low, so the cell edges can be approximated as thin beams. Beams *a priori* can be naturally curved and have non-uniform cross-sections, as long as the cross-sectional area $s_{ij}(l)$ of each beam (i,j) (where l refers to the curvilinear coordinate along the beam, and i and j denote the two nodes

linked by the beam) is small compared with its length l_{ij} squared. Let us isolate a circular portion of this material, of radius R, and impose a uniform radial displacement $-\delta R\mathbf{e}_r$ on its boundary ($\mathbf{e}_r$ is the radially oriented unit vector; the body is under uniform tension when $\delta R < 0$, and under uniform compression when $\delta R > 0$, see Fig. 1). We define the 2D bulk modulus $\kappa^{(2D)}$ of this structure as:

$$\frac{1}{\kappa^{(2D)}} = \frac{1}{\pi R^2}\frac{2\pi R\delta R}{\delta P} = \frac{2}{R}\frac{\delta R}{\delta P}, \tag{3}$$

where δP is the average load applied on the boundary. We must point out that the definition above is different from the usual definition of bulk modulus: in the usual definition, a uniform radial *load* is applied on the surface of the material, while in the present definition a uniform *displacement* is imposed on its surface (allowing to extend the notion of bulk-modulus to non-isotropic materials). However, the two definitions are identical for 2D materials with square or hexagonal symmetry and for 3D materials with cubic or isotropic symmetry.

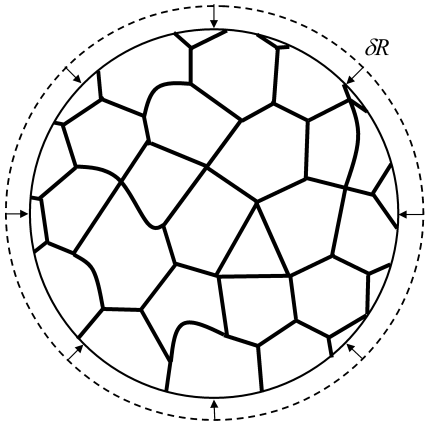

FIG. 1: Circular portion of a 2D cellular network subjected to a uniform radially oriented displacement $-\delta R\mathbf{e}_r$ of its boundary. The network is made of thin beams with *a priori* natural curvatures and non-uniform cross-sections. We associate a bulk modulus for such a strain, defined as: $\kappa^{(2D)} = \frac{R}{2}\frac{\delta P}{\delta R}$, where δP is the average load applied on the boundary.

The expression of an upper bound can be easily established using the principle of minimum potential energy: *among all kinematically admissible displacement fields (i.e. any displacement field twice continuously differentiable satisfying the displacement constraints on the boundary), the actual displacement (i.e. the one satisfying the equations of mechanical equilibrium) is the one that makes the potential energy an absolute minimum.* Let $\mathbf{u}^*(\mathbf{r})$ be the displacement field which satisfies the equations of equilibrium throughout the body and the conditions on the boundary, $\mathbf{u}(\mathbf{r})$ any kinematically admissible displacement field, and $U(\{\mathbf{u}^*(\mathbf{r})\})$ and $U(\{\mathbf{u}(\mathbf{r})\})$ the respective potential energy associated with these two displacement fields. Then, according to the principle of minimum potential energy:

$$U(\{\mathbf{u}^*(\mathbf{r})\}) \leq U(\{\mathbf{u}(\mathbf{r})\}). \tag{4}$$

Let us choose as kinematically admissible displacement field: $\mathbf{u}(\mathbf{r}) = -\frac{\delta R}{R}\mathbf{r}$, and let us evaluate the potential energy associated with. We assume the cross-section of each beam is sufficiently small so $\mathbf{u}(\mathbf{r})$ is uniform on it (or equivalently, we suppose $\mathbf{u}(\mathbf{r})$ is a macroscopic field which has a uniform value on the beam cross-section). Thus, the stress tensor expressed in the local orthogonal coordinate system has only one non-zero component: the axial-axial component. Consider an infinitesimal piece of a given beam (i,j), of length dl and cross-sectional area $s_{ij}(l)$. We denote $\mathbf{r}_M$ and $\mathbf{r}_M+d\mathbf{r}$ the position of its two ends. Their relative displacement $(\mathbf{u}(\mathbf{r}_M+d\mathbf{r}) - \mathbf{u}(\mathbf{r}_M))$ is colinear to the local tangent unit vector $\mathbf{t}_{ij} = \frac{d\mathbf{r}}{dl}$, meaning that the piece of beam deforms by axial compression only. The force $\mathbf{F}_{ij}(l)$ acting on the surface $s_{ij}(l)$ is parallel to $\mathbf{t}_{ij}$ and given by: $\mathbf{F}_{ij}(l) = Es_{ij}(l)\frac{\delta R}{R}\mathbf{t}_{ij}$, where E is the Young modulus of the solid phase. The strain energy associated with such a deformation is $\frac{E}{2}s_{ij}(l)\left(\frac{\delta R}{R}\right)^2$. Invoking additivity of the potential energy :

$$U(\{\mathbf{u}(\mathbf{r})\}) = \sum_{(i,j)}\int_0^{l_{ij}}\frac{E}{2}s_{ij}(l)\left(\frac{\delta R}{R}\right)^2 dl \tag{5}$$

(where the discrete sum is carried out on all the beams (i,j)), and introducing the volume fraction of solid:

$$\phi = \sum_{(i,j)}\int_0^{l_{ij}} s_{ij}(l)dl/\pi R^2, \tag{6}$$

we obtain:

$$U(\{\mathbf{u}(\mathbf{r})\}) = \frac{\pi}{2}E\phi(\delta R)^2. \tag{7}$$

On the other hand, the actual potential energy $U(\{\mathbf{u}^*(\mathbf{r})\})$ is equal to half the work done by the external forces [13]:

$$U(\{\mathbf{u}^*(\mathbf{r})\}) = \frac{1}{2}\delta P 2\pi R\delta R = 2\pi\kappa^{(2D)}(\delta R)^2. \tag{8}$$

Comparison of Eqs. 7 and 8 finally leads to an upper-bound for the bulk modulus:

$$\kappa^{(2D)} \leq \frac{E\phi}{4}. \tag{9}$$

The same argumentation can be used for 3D open-cell structures: in that case, we find that the bulk modulus $\kappa^{(3D)}$ associated with a spherical portion of material of radius R, and defined as:

$$\frac{1}{\kappa^{(3D)}} = \frac{1}{\frac{4}{3}\pi R^3}\frac{4\pi R^2\delta R}{\delta P} = \frac{3}{R}\frac{\delta R}{\delta P}, \tag{10}$$

is bounded as it follows:

$$\kappa^{(3D)} \leq \frac{E\phi}{9}. \tag{11}$$

The upper-bound value we obtain is then lower than the HS upper-bound value 2, giving a sharpest estimation of the actual bulk modulus value.

Criteria for maximal bulk modulus

The upper bounds established above are optimal bounds, i.e. there exist cellular materials with maximal bulk modulus value. Criteria on the structure of such materials can be provided. Indeed, we show in the following that the bulk modulus equals the upper-bound value *if and only if* the three following conditions are simultaneously satisfied:

a) All the edges are straight.

b) Each edge has a uniform cross-section area: $s_{ij}(l) = s_{ij}$.

c) Every junction (i) between edges satisfies $\sum_j s_{ij}\mathbf{e}_{ij} = \mathbf{0}$, where $\mathbf{e}_{ij}$ are outward-pointing unit vectors in the directions of adjoining edges.

The demonstration is straightforward: according to the principle of minimal potential energy and the uniqueness of the actual displacement field, the inequality 4 becomes a strict equality if and only if the trial displacement field $\mathbf{u}(\mathbf{r}) = -\frac{\delta R}{R}\mathbf{r}$ is the actual displacement field satisfying the equations of mechanical equilibrium. Inspection of force and moment balances along each beam and at each junction leads to the three necessary and sufficient conditions stated above. Let us make this precise. Consider a specific beam (i,j) (see Fig. 2); at equilibrium, the moments of forces acting on it must balance. Choosing as referencing point for the moments the node i, and denoting $\mathbf{r}_{iM} = \mathbf{r}_M - \mathbf{r}_i$, where $\mathbf{r}_i$ and $\mathbf{r}_M$ are the respective position vectors of node i and of any point M belonging to the beam, we obtain: $\mathbf{r}_{iM} \times \mathbf{F}_{ij}(l) = Es_{ij}(l)\frac{\delta R}{R}\mathbf{r}_{iM} \times \mathbf{t}_{ij} = \mathbf{0}$. Thus, the tangent unit vector $\mathbf{t}_{ij}$ must be parallel to the position vector $\mathbf{r}_{iM}$ for any point M belonging to the beam, leading to condition a). The forces acting on any piece $\triangle l$ of the straight beam (i,j) must balance as well: $E\frac{\delta R}{R}s_{ij}(l) = E\frac{\delta R}{R}s_{ij}(l+\triangle l)$ what immediately leads to condition b). Finally, mechanical equilibrium at every junction i is satisfied if: $\sum_j \mathbf{F}_{ij} = \mathbf{0}$, with $\mathbf{F}_{ij} = -Es_{ij}\frac{\delta R}{R}\mathbf{e}_{ij}$, leading to condition c). The moment balance at every junction is automatically satisfied when conditions a), b), c) are fulfilled, since the force acting on each straight beam is then axially oriented. Furthermore, we check that the geometrical constraint on angles between adjoining edges is also satisfied; if $\mathbf{e}'_{ij}$ denotes the unit vector parallel to the beam (i,j) *after* deformation and $\mathbf{r}_{ij} = \mathbf{r}_j - \mathbf{r}_i$, then:

$$\mathbf{e}'_{ij} = \frac{\mathbf{r}_{ij} + \mathbf{u}(\mathbf{r}_j) - \mathbf{u}(\mathbf{r}_i)}{\|\mathbf{r}_{ij} + \mathbf{u}(\mathbf{r}_j) - \mathbf{u}(\mathbf{r}_i)\|} = \frac{\left(1 - \frac{\delta R}{R}\right)\mathbf{r}_{ij}}{\left(1 - \frac{\delta R}{R}\right)\|\mathbf{r}_{ij}\|} = \mathbf{e}_{ij}, \tag{12}$$

what proves the material deforms by affine compression, and the angles between edges are preserved.

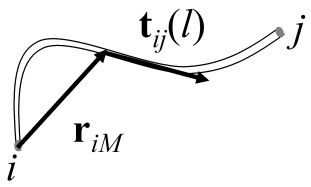

FIG. 2: Schematic of a paticular beam (i,j). l denotes the curvilinear coordinate of a given point M along the beam. $\mathbf{r}_{iM}$ and $\mathbf{t}_{ij}$ are respectively the position vector of point M taken from node i and the local tangent unit vector.

Some comments

We first summarize the limits of the theory: the solid volume fraction is supposed to be low enough for the thin beam theory to be valid. Moreover the relative imposed displacement $\frac{\delta R}{R}$ must be small enough so that Hooke's law can be used and no mechanical Euler instability occurs when the body is under compression.

Conditions a), b), c) are the necessary and sufficient conditions to maximize the average conductivity of a network of thin wires as well [12]. Why structures satisfying these conditions have both maximal bulk modulus and maximal conductivity ? When the three conditions are fulfilled, the force acting to each beam is then parallel to it, and the corresponding deformation of each beam is an axial compression (or tension); no bending or twisting occurs. The "flow" of stress is parallel to the beams, as for the electric courant, and the geometry defined by the three conditions corresponds to the most homogeneous distribution of constraints and currents through the whole structure.

We must point out that condition c) is sufficient for having no bending in a structure for which conditions a) and b) are fulfilled, but not necessary: there do exist structures which do not satisfy condition c) and which deform under compression without bending (e.g. see structures of Fig. 3). Nevertheless, the bulk modulus of such structures will be below the upper-bound value; condition c) must be satisfied in order to have maximal bulk modulus.

Furthermore, it is worth noticing that the three conditions are independent of the connectivity of the junc-

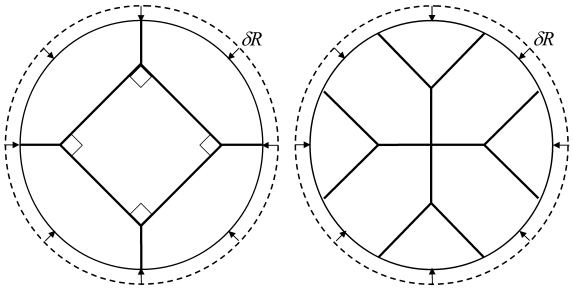

FIG. 3: Examples of cellular networks for wich condition c) is not satisfied and still deform by affine compression (no bending or twisting of the beams). However their respective bulk modulus is strictly lower than the upper bound value $\frac{E\phi}{4}$.

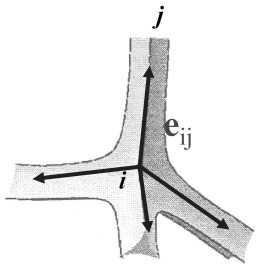

FIG. 4: In a real 3D foam, the edges (also called Plateau borders) meet in fourfold junction with equal angles, corresponding to the tetrahedral angle: $\arccos\left(-\frac{1}{3}\right) \simeq 109,5°$.

tions. As a consequence, there is an infinity of structures with maximal bulk modulus. Indeed, various examples of structures with maximal bulk modulus can be found in literature: we can cite the square, hexagonal, triangular, kagomé networks [9][10] as 2D structures and the cubic [2] and Kelvin networks [4][5][14] as 3D structures. All these structures satisfy the necessary and sufficient conditions a), b), c), in agreement with the work presented here. Numerical simulations of random 2D [9][15] and 3D [16] isotropic cellular materials have been also generated. As expected, the bulk modulus of those materials is found to be always lower than the respective upper bound values.

As concluding remarks, let us discuss the consequences of the criteria presented here on the mechanical properties of real foams. Foam in the low-density limit is a particular cellular material: usually its preparation involves a continuous liquid phase that eventually solidifies. Therefore its structure is controlled by minimization of surface energy, leading to geometrical rules known as the Plateau's laws [1], which can be summarized as it follows:

- edges in a 2D foam meet in threefold junctions with equal angles of 120°.

- lamellae in a 3D foam meet in threefold lamella junctions (usually called Plateau borders) with equal angles of 120°, and Plateau borders meet in fourfold junctions with the tetrahedral angle: $\arccos\left(-\frac{1}{3}\right) \simeq 109,5°$ (see Fig. 4).

As a consequence, condition c) is always satisfied in a real foam. Usually, condition b) is nearly satisfied as well. The validity of condition a) is more delicate: while it is still possible to build 2D foams satisfying simultaneously conditions a), b), c) and the Plateau's laws (e.g. the hexagonal honeycomb), this is no longer true for the 3D case: no cell in a 3D foam is a simple polyhedron with straight edges, because a planar polygon cannot have all angles equal to the tetrahedral angle. Consequently, edges in a real foam must be curved, violating condition a), and the bulk modulus and the average conductivity of a solid open-cell foam (i.e. a foam where the lamellae broke up during solidification) is always strictly lower that the corresponding bounds. While the conductivity drop is not really significant when the edges are slightly curved [11], the bulk modulus value can be dramatically decreased, because beams can easily bend or twist. We conclude that 3D cellular materials manufactured by some foaming process are probably not the most relevant for the design of high-bulk modulus/low-density structures.

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