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Explicit effective elastic moduli for anisotropic triply periodic frame networks

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Abstract

We derive analytical expressions for the effective elastic moduli of periodic tetrahedrally coordinated frame networks with an arbitrary Bravais lattice without recourse to matrix inversion. Previously, this was only possible for isotropic or hexagonal structures. Crown Copyright \odot 2007 Published by Elsevier B.V. All rights reserved.

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1. Introduction

Cellular networks, foams, lattices, crystals (both regular and irregular) appear widely in both technology and nature. Much of the technologically motivated literature is concerned with analysing and designing structures with certain optimal properties (bulk modulus, conductivity, band gaps). Naturally occurring cellular materials such as cork, wood and bone are also of practical importance and the presence of many types of two-dimensional and threedimensional networks within biological cells is of interest to biologists and biophysicists.

Certainly, sophisticated numerical algorithms exist that can calculate the mechanical properties of complicated and arbitrary structures. There is also an extensive literature over four decades that concerns itself with establishing bounds for structures with given volume fraction [\[1,2\].](#page--1-0) Optimal structures that achieve these bounds are known in many cases and some interesting, necessary conditions for the physical attributes of these structures are also known. For example, for open cell foams, optimal bulk moduli are attained by networks where all the individual beams compress without bending [\[3\];](#page--1-0) this occurs for orthorhombic

structures with beams that are straight with uniform crosssections such that the volumes of the beams in each of the orthogonal directions are equal [\[4\].](#page--1-0) The simple cubic lattice is the most symmetric of such structures. Similarly, optimal shear moduli are attained in analogous diamond-like structures where the volume of beams in each of four mutually equally inclined directions are equal [\[4\].](#page--1-0) The fcc lattice with equal beams is the most symmetric of these latter structures.

Explicit expressions for the moduli of the simplest and most symmetric structures are known (though often certain simplifying mechanical assumptions are needed) [\[5,6\].](#page--1-0) There has been less published on structures of lower symmetry [\[7\]](#page--1-0). Lattices of low symmetry are gaining more attention in studies of self-organising complex biological structures [\[8\].](#page--1-0) Results for such crystal lattices, will help unravel the structure–function relationship of these interesting objects.

In this paper, we are interested in obtaining explicit analytical results for systems which are periodic. We look at how the properties of a system vary as the periodic lattice changes. Most of these structures will not be optimal and in this paper we do not explore bounds or other effective medium approximations. In order to make analytical progress we limit our structures to frame networks.

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A frame network is a particular type of network of joints and struts where the struts are assumed to be deformable (they can stretch, bend and twist) but the joints are assumed to be rigid (they can translate or rigidly rotate but the angles at which the struts meet at a joint are fixed). The elastic properties of many biological networks have been successfully explained using the frame model [\[9,10\]](#page--1-0). Thus, apart from the assumptions mentioned in this paragraph and St. Venant's principle (see later), the remaining analysis is exact.

Arbitrary frame networks can always be analysed by solving the simultaneous equations that arise from forces producing deformations. However, explicit analytical results have until now been limited to networks which are both isotropic and periodic (the simple cubic and diamond structures [\[5\]](#page--1-0) and a structure made from tessellating Kelvin polyhedra [\[6\]](#page--1-0)). The hexagonal structure can also be analysed in this way because it is isotropic in the transverse plane [\[7\].](#page--1-0)

We start by describing the geometry of the unit cell and introducing appropriate notation for the various vectors (lattice vectors, reciprocal vectors and strut vectors). We then proceed to derive relationships for the effective stress and strain using properties at the level of a unit cell. We then show how these expressions can be reformulated in terms of the struts inside the unit cell. Finally, we combine these results with a microscopic model of the deformations based on Euler–Bernoulli beam theory.

We close the paper with an example application where we vary the length and angle of the struts in such a way as to continuously deform our lattice through a family of structures exhibiting different symmetries.

2. The unit cell

We build a network by tessellating an arbitrary tetrahedrally coordinated joint: one where each of the four struts can have a different length (and other properties) and meet the other struts at arbitrary angles. The only restriction is that the four struts are not coplanar. Let the four vectors representing these struts be denoted \mathbf{b}^i for $i = 0, \ldots, 3$. We use superscripts to distinguish one vector from another since we wish to reserve the subscripts for indicating Cartesian components. If we look at all possible differences between these four strut vectors we see that there are only three of them that can be linearly independent. We choose $\mathbf{a}^i = \mathbf{b}^i - \mathbf{b}^0$ for $i = 1, ..., 3$ to be the three we use. When this single joint is tessellated to fill all space a periodic structure with lattice vectors a^i is formed. Thus, any crystal Bravais lattice can be obtained in this way.

Since the four struts that meet at each joint have arbitrary dimensions the network need not have any rotation or reflection symmetries about the centres of these joints. The individual joints may even be chiral. However, and surprisingly, the network is not chiral, and is centrosymmetric about the midpoint of any strut. This result can be obtained fairly easily from the relationship between the vectors a and b. If in addition we take the origin to be located about the centre of the strut represented by \mathbf{b}^0 and construct a primitive unit cell centered on this point, then we discover that the midpoints of the other three struts (labelled 1–3) will intersect the faces of the unit cells at their midpoints. The resulting standard configuration is shown in Fig. 1.

The structure shown is obviously tetrahedrally coordinated. However, structures with six-fold coordination but arbitrary lattices can be obtained from these structures by taking the limit where the strut \mathbf{b}_0 vanishes. In this limit strut vectors and lattice vectors become the same.

3. Equilibrium and homogeneous deformations

It is useful to introduce a triplet of vectors which are reciprocal to the lattice vectors. If V is the volume of the unit cell then we choose our reciprocal vectors A^{α} to satisfy

$$
a^{\alpha} \cdot A^{\beta} = V \delta^{\alpha \beta}.
$$
 (1)

This choice of normalisation is useful since A^{α} can also be identified with the area vectors of the faces of the unit cell.

We ignore rigid translations and rotations of the unit cell and consider only homogeneous deformations; these can be expressed by giving the deformations Δ^{α} corresponding to each of the primitive lattice vectors a^{α} for $\alpha = 1, \ldots, 3$. The absence of rigid rotations is given by the requirement

$$
\sum_{\alpha=1}^{3} \varDelta^{\alpha} \times \mathbf{A}^{\alpha} = 0. \tag{2}
$$

In equilibrium the net forces acting on opposite faces of the unit cells must balance and we label these F^{α} . The absence of a net torque in equilibrium is given by the requirement

$$
\sum_{\alpha=1}^{3} \mathbf{a}^{\alpha} \times \mathbf{F}^{\alpha} = 0.
$$
 (3)

Fig. 1. Each unit cell contains exactly two mirror image tetrahedral joints. The midpoints of each strut line up with the midpoints of the faces. The small arrows show the forces acting on the faces of each unit cell.

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