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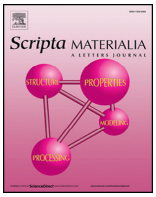

Conductivity and Young's modulus of porous metamaterials based on Gibson-Ashby cells

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ABSTRACT

The effective conductivity and Young's modulus of metamaterials based on Gibson-Ashby cells have been calculated numerically. It is shown that the porosity dependences of these properties do not follow the Gibson-Ashby relations for open-cell foams, although the latter have been derived on the basis of this model. For low-porosity metamaterials with porosity 0.016 the relative conductivity and Young's modulus are still as low as 0.80 and 0.65, respectively. It is shown that these low relative property values are caused by the strongly oblate shape of the pores, which become microcrack-like voids as zero porosity is approached.

The Gibson-Ashby relation for three-dimensional strut-based cellular materials (for high-porosity called open-cell foams), which can be written as

$$k_r = (1-\varphi)^{3/2} \tag{1}$$

for conductivity (thermal or electrical) [1] and

$$E_r = (1-\varphi)^2 \tag{2}$$

for Young's modulus [1,2], is one of the most frequently cited microstructure-property relations for porous and cellular materials. In these equations φ is the porosity, i.e. the volume fraction of the void space, k_r the relative conductivity, i.e. the non-dimensional ratio of the effective conductivity of the cellular material and that of the dense (pore-free) solid, and E_r the relative Young modulus, i.e. the ratio of the effective Young modulus of the cellular material and that of the dense solid. Indeed, the Gibson-Ashby relations are probably the most successful predictive relations for the effective properties of high-porosity cellular materials with porosities higher than 70%, so-called solid foams.

Recent numerical calculations on digital microstructures representing different types of model foams or, more generally, strut-based and wall-based cellular (meta-)materials [3], have shown that these Gibson-Ashby relations provide excellent predictions for periodic strut-based (open-cell) metamaterials with Kelvin cells, whereas the properties of the corresponding random metamaterials, i.e. cellular materials with randomly arranged cells that are neither regular nor semiregular polyhedra (open-cell random foams) are usually significantly below these predictions. On the other hand, it has been found [3], that in the case of sufficiently low porosities these Gibson-Ashby relations, which have originally been derived for open-cell foams [1,2], provide excellent predictions also for closed-cell foams (or, more generally, for wall-based metamaterials), both periodic (with Kelvin cells) and random (with random cells), although the latter are completely different from the viewpoint of topology. Actually, in contrast to the former, the latter correspond to a matrix-inclusion microstructure, since the void cells are always simply connected and isolated, i.e. well separated from their neighbors by the solid phase. Moreover, it has been shown recently [4], that – in contrast to common belief – in the case of porous materials with random microstructures based on convex spherical pores the Gibson-Ashby relation provides better predictions for isolated pores (i.e. closed cells) than for overlapping pores (i.e. open cells). These apparently paradoxical and for many readers probably unexpected results should not be considered as being too surprising. They just confirm the tentative character of the Gibson-Ashby predictions, which is of course a feature that these relations share with most other predictive relations and effective medium approximations [5–7], including the Pabst-Gregorová exponential relations for conductivity and Young's modulus [8,9].

Much more surprising, however, is the fact that – to the best of our knowledge – results of numerical calculations of the effective properties of cellular metamaterials based on the Gibson-Ashby cell (in the sequel

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abbreviated as "GA cell"), i.e. virtual materials with digital microstructures that correspond exactly to the Gibson-Ashby model, have never been published so far. We will show in the sequel that the results of these calculations are indeed quite remarkable and prove that – in contrast to widespread belief – the porosity dependence of properties for strut-based (i.e. open-cell) metamaterials based on GA cells actually cannot be described by the aforementioned Gibson-Ashby relations.

A potential pitfall when attempting to generate cellular materials (metamaterials) based on GA cells arises due to the fact that the original GA cell, as sketched in [1] and many times reproduced in the literature, see Fig. 1a, is not suitable for this purpose. Actually, it is impossible to construct a three-dimensional (3D) cellular material (metamaterial) based on this original GA cell, because the interconnecting struts for the third dimension (perpendicular to the other four pairs of struts) are missing. Only planar structures with finite thickness (sometimes called "2.5-dimensional"/"2.5D"), can be generated using the original, incomplete GA cells, see Fig. 1c. By contrast, Fig. 1d shows a 3D open-cell metamaterial based on the complete GA cell to which these two pairs of struts (normal to the paper plane) have been added, see Fig. 1b (see also Ashby's later contributions, e.g. [10]). Note in passing, that 3D wall-based (closed-cell) metamaterials based on closed GA cells, as sketched in [1], do not exist and that the "2.5D" version of these materials does not consist entirely of closed cells, see Fig. 1e. This is the reason why only strut-based (open-cell) metamaterials can be considered in this paper and why wall-based (closed-cell) metamaterials have to be ignored.

Both the generation of the digital microstructures (virtual metamaterials) and the calculation of the effective properties has been performed in this work with the help of the commercial software package GeoDict® (Math2Market, Germany). GA cells based on struts with square cross sections have been constructed in cubic boxes (unit cells) with 200 × 200 × 200 cubic voxels, using the GridGeo module of GeoDict®, resulting in periodic metamaterials with void volume fractions ranging from 0.016 to 0.999 (achieved by changing the strut thickness). The effective thermal conductivity tensor has been calculated using the ConductoDict module of GeoDict®, which relies on a solver based on the so-called explicit jump immersed interface method [11,12], whereas the effective elastic tensor (stiffness matrix) has been calculated using the ElastoDict module of GeoDict®, which is based on an iterative solution, assisted by fast Fourier transform, of the Lippmann-Schwinger equation [13,14]. The temperature gradient and deformation imposed were 2 K and 0.005, respectively, in the direction the field to be calculated. Periodic boundary conditions were imposed in all directions for both conductivity and elasticity calculations, so that the results hold for the metamaterial consisting of an infinite number of unit cells and not for a single unit cell body. Compared to the pore phase, the solid phase was assumed to have a conductivity higher by more than three orders of magnitude (corresponding, e.g., to the thermal conductivity of dense polycrystalline alumina with air-filled pores at room temperature, as in our previous papers [3,4]), so that the pore phase conductivity (taken to be 0.026 W/mK) is completely neglible with respect to the solid phase conductivity (taken to be 33 W/mK). The Young's modulus of the pore phase (void space) has been set to zero, which is tantamount to assuming the Young's modulus of the solid phase (taken to be 400 GPa) to be infinitely high compared to the pore phase (void space). Of course, both for conductivity and for Young's modulus the absolute values are irrelevant in this work, because all data have been normalized with respect to the property value of the dense solid phase, resulting in (dimensionless) relative properties. The Poisson ratio has been varied from +0.49 (almost incompressible solid phase) to – 0.99 (extremely auxetic solid phase), in order to produce material-independent results of universal validity, although the practical focus of this work is on metamaterials with a compressible and non-auxetic solid phase, which can be readily produced from common solid material powders via additive manufacturing (3D printing) techniques. From the viewpoint of symmetry, 3D metamaterials based on GA cells are cubic. Therefore the conductivity tensor is naturally isotropic. By contrast, in order to obtain quasi-isotropic elastic constants from the cubic stiffness matrix, Voigt-Reuss-Hill averaging has been used [15]. In other words, these values correspond to a quasi-isotropic material, consisting of randomly oriented GA-cell-based "metacrystallites".

Fig. 1f through 1j show strut-based (open) GA cells with different porosity (void space fraction in the unit cube). It is evident that the high-porosity (thin strut) case corresponds more or less to the three-point bending mechanism assumed by Gibson and Ashby [1,2], whereas the low-porosity (thick strut) case leads to strongly anisometric pores. Actually, in the extreme case approaching infinitely thin struts (i.e. in practice 1D struts consisting of single-voxel chains) an ideal (long slender beam) three-point bending situation is approached, as envisaged by Gibson and Ashby [1,2], whereas the opposite extreme case approaching infinitely thin oblate pores (in practice 2D voids with two-voxel thickness) the metamaterial can be considered as a model structure for a material with microcracks.

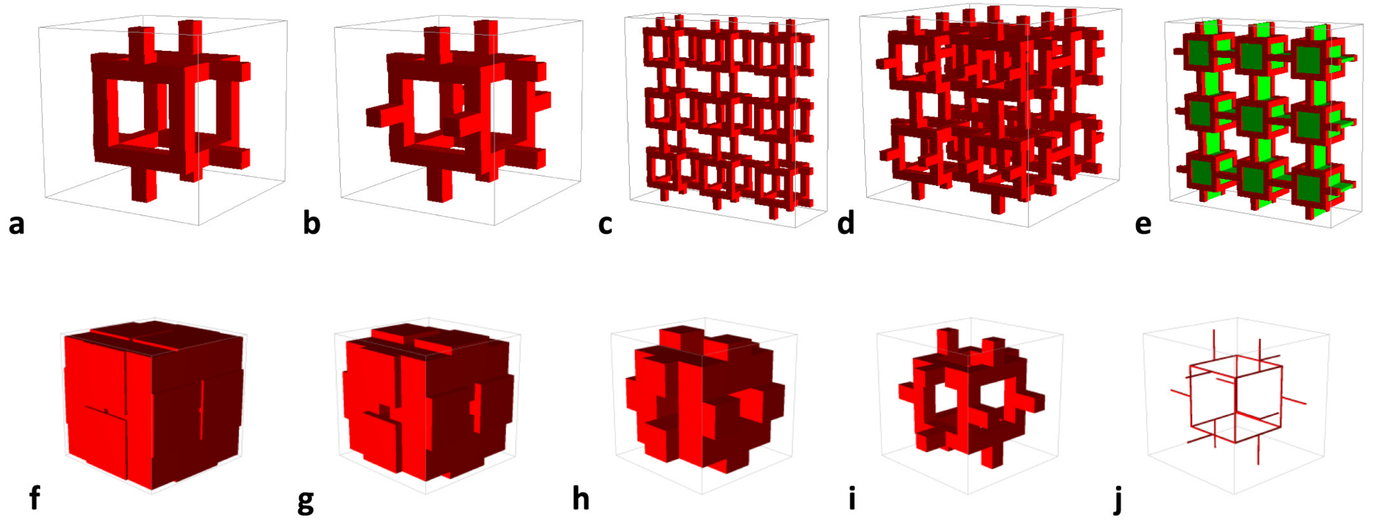

Fig. 1. Two versions of the open Gibson-Ashby cell (GA cell), viz. original open GA cell (not suitable for modeling 3D metamaterials due to missing struts in the third dimension), see [1] (a), and complete GA cell, see [10] (b), strut-based (open-cell) metamaterials (2.5D) based on the original (incomplete) open GA cell, see [1] (c), strut-based (open-cell) metamaterials (3D) based on the complete open GA cell, see [10] (d), and wall-based (partly closed-cell) metamaterials (2.5D) based on the original closed GA cell proposed in [1] (e), and strut-based (open) GA cells with different porosity (void space fraction in the unit cube, bottom row from left to right): 0.07 (f), 0.25 (g), 0.59 (h), 0.89 (i), 0.999 (j).