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Scale-size effects analysis of optimal periodic material microstructures designed by the inverse homogenization method

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ABSTRACT

Periodic homogenization models are often used to compute the elastic properties of periodic composite materials based on the shape/periodicity of a given material unit-cell. Conversely, in material design, the unit-cell is not known *a priori*, and the goal is to design it to attain specific properties values – inverse homogenization problem. This problem is often solved by formulating it as an optimization problem. In this approach, the unit-cell is assumed infinitely small and with periodic boundary conditions. However, in practice, the composite material comprises a finite number of measurable unit-cells and the stress/strain fields are not periodic near the structure boundary. It is thus critical to investigate whether the obtained topologies are affected when applied in the context of real composites. This is done here by scaling the unit-cell an increasing number of times and accessing the apparent properties of the resulting composite by means of standard numerical experiments.

1. Introduction

The optimal design of materials with periodic microstructure to achieve specific properties has been a major area of interest in materials research [1]. The so-called "unit-cell" is the microstructure representative of the smallest periodic heterogeneity of the material domain. The material is then defined assembling unit-cells, i.e. repeating the unit-cell in all directions of the space.

Periodic cellular composites are so attractive because they offer great flexibility in tailoring different physical properties by controlling the microstructural architecture in unit-cells and they can be realized by additive manufacturing technologies [2]. This has opened the way to explore and develop novel multi-functional composites even to the point of exhibiting exceptional properties usually not encountered in nature – metamaterials [3].

To take full advantage of the possibilities provided by these materials systematic design methods are required. The inverse homogenization method is often used for this purpose [4]. The goal is to design the unit-cell targeting prescribed effective (homogenized) properties or extremizing a function of those properties (e.g. strain energy). This can be solved by designing the unit-cell through topology optimization [5]. Material type or density in each element of the finite element mesh discretizing the unit-cell serves as the design variable and hence, the design freedom is huge allowing for exceptional improvements on material efficiency.

A thorough review of periodic microstructure design using inverse homogenization supported on topology optimization was carried out by Cadman et al. in 2013 [1]. Further advances in the design of periodic microstructures of multi-functional materials for a range of physical properties have been published in the meantime which proves how active this research area has been. For instance, quite recent research papers present optimal material designs for poroelastic actuators [6], elastic stiffness [7–11], Poisson's ratio [2,9], natural frequencies [12], thermal conductivity [10], fluid permeability [11], negative or zero compressibility [13], viscoelastic behavior [14–16], bone scaffolds [17], piezocomposites [18,19].

The inverse homogenization method assumes that the scale of a unit-cell is indeterminate (infinitely small) as well as periodic Boundary Conditions (BC's) [20–23]. This makes uncertain whether the obtained topology can be translated into real composites of macroscale. In practice, one has a finite number of measurable unit-cells assembled together to define the composite sample. Moreover, the stress or strain fields are in general arbitrary (not periodic) near the boundary of the composite.

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Therefore it is critical to investigate how the apparent properties of the composite converge as one scales the unit-cell an increasing number of times. Numerical standard experiments based on BC's of uniform stress and strain can be applied to access the apparent properties of the resulting composite for a specific scale factor [24]. This factor is defined here as the ratio between the linear size of the composite and the linear size of the unit-cell. As this factor increases one may evaluate convergence of the apparent properties to the theoretical values from homogenization. This scale-size effects analysis has been carried out by other authors although restricted to material symmetries, mostly to two-dimensional microstructures and investigating mainly the convergence of the mean compliance, few elastic moduli and fundamental frequency [25–32]. The aim of the present work is to extend this to three-dimensional anisotropic material microstructures. This paper is based upon Coelho et al. [33], but the current paper adds the full apparent elasticity tensor estimate based on additional numerical experiments, measures the degree of microstructural anisotropy, investigates convergence on more elastic tensor coefficients as well as on strain/stress energy density and increases also the scale factor from 5 to 6.

Ideally a convergence analysis of optimal periodic microstructures would be carried out, from the finite periodicity to the theoretically infinite periodicity. This extreme case is of course practically infeasible. Due to the limitation of the computational resources available, only a few low scale factors have been tried for three-dimensional analyses. Despite this analysis limitation, the outcome of this study indicates that it is sufficient to have a low scale factor to replace the non-homogeneous composite by the equivalent homogeneous material with the moduli computed by homogenization. This is demonstrated here with material microstructures that extremize elastic stiffness considering different load cases and subjected to either volume fraction or permeability constraints. For the unit-cell topologies selected, one studies ultimately how rapidly the 21 independent elastic coefficients from the apparent fourth-order stiffness tensor converge to the corresponding values of the homogenized stiffness tensor.

2. Materials and methods

2.1. Material model

The material model here is a three-dimensional porous composite material (solid-void phases) generated by the repetition of a unit-cell in all directions of the space. The unit-cell represents the smallest periodic heterogeneity of the composite domain Ψ whose material properties are calculated by homogenization. This theory assumes periodic boundary conditions (BC's) applied to the unit-cell domain Y and infinite periodicity of the unit-cell (Y-periodic), i.e. its feature size d is much smaller than the cellular material global size D ($d/D \to 0$), see Fig. 1.

In the case of optimal material design, the design domain is the unit-cell domain Y. Ideally, one would determine the pointwise material distribution in this domain that optimizes the design goal. In practice, the true pointwise material distribution cannot be found, but one can discretize the domain Y with a large number of finite elements and let the density μ in each element be a variable. Here one uses a regular mesh $20 \times 20 \times 20$ of 8-node isoparametric hexahedral finite elements as shown in Fig. 1. Solid and void phases correspond to μ equal to 1 and 0, respectively. Topology optimization can then be used to search for an optimal material microstructure layout targeting desired effective properties. This design method is also known as inverse homogenization and it was originally introduced by Sigmund [4]. The effective material properties (homogenized) can be found using a numerical homogenization procedure described in [23].

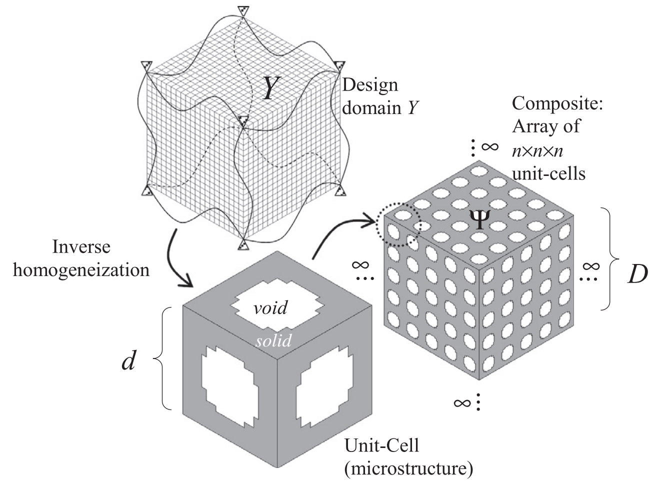

Fig. 1. Material model of solid-void composite. Discretization of Y with periodic BC's. Array of $5 \times 5 \times 5$ unit-cells of global size D (in theory goes to infinity) and one unit-cell of size d.

2.2. Optimization problem

In this work one extremizes an energy density based objective function subjected to a minimum prescribed permeability of the material microstructure in all directions of the space. Such a problem is of practical interest, for example, to design scaffolds for skeletal Tissue Engineering. Ensuring isotropic permeability in scaffolds favors the migration of cells, nutrients and waste products needed for native tissue regeneration while ensuring a preferential stiffness direction helps the scaffold fulfilling its rule as a load bearing device. An appropriate trade-off between these two conflicting properties, permeability (favors porosity) and stiffness (favors density), can be achieved through topology optimization [11,34–39]. The local anisotropic material design problem can be then defined by Eq. (1) and a brief description is given below (for full details see e.g. [33,35,40,41]).

$$\begin{aligned} &\min_{\mu} \quad \frac{1}{2} C^{H}_{mnkl}(\mu)\overline{\sigma}_{mn}\overline{\sigma}_{kl} \\ &\text{subject to:} \\ &K^{H}_{ij}(\mu) \geqslant k^{*}; \quad i=j=1,\ldots,3 \\ &K^{H}_{ij}(\mu) = 0; \quad i \neq j \text{ and } i,j=1,\ldots,3 \end{aligned} \tag{1}$$

In Eq. (1) μ is the local density varying between 0 (void) and 1 (material) which depends on the spatial variable y in the unit-cell design domain Y (see Fig. 1). The problem is formulated for the minimization of the stress energy density or mean compliance. The stress tensor is $\overline{\sigma}$ and characterizes an averaged macroscopic stress field applied to the composite which is here fixed *a priori* (e.g. hydrostatic). The homogenized compliance tensor is $\mathbf{C}^{H}$, i.e. the inverse of the homogenized stiffness tensor $\mathbf{E}^{H}$. The stiffness tensor at each point of Y is related to the tensor $\mathbf{E}^{0}$ of the base material properties through the SIMP interpolation scheme [42]. Regarding the optimization problem constraints, one enforces the permeability tensor to be diagonal and each diagonal coefficient has to be "equal" or "greater than" a threshold, k^{*}. This way one gets an interconnected pore network on the periodic material satisfying a critical (minimum) permeability in all direction of the space. The permeability measure of porous media is given by the homogenized tensor $\mathbf{K}^{H}$. This tensor is obtained homogenizing a potential flow problem in periodical porous media characterized by the Darcy law [20,22]. Here one considers the interpolation between permeability and local density μ given by a power-law