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Numerical and experimental study on effective elastic properties of porous materials: controlled porosity numerically generated and 3D printed.

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Abstract — This work aims to introduce a methodology for the determination of the effective properties of random heterogeneous materials. Specifically, focus of this study are the effective properties of two phase porous material containing spherical voids which are investigated both experimentally and numerically. To this end, three-dimensional porous structures, with non-overlapping porosity, are first generated by means of a random sequential algorithm. Numerical simulations are conducted on a representative volume element, whose size is first determined. Specimens are fabricated by 3D-printing of the computer-generated microstructures and tested under uniaxial loading. Good agreement of Young modulus data is found, in the case of spherical monodisperse porosity.

Keywords: — Representative volume element, heterogeneous materials, 3D printed materials.

1. Introduction

Heterogeneous media combine multiple monomineralic phases. These materials are largely abundant in nature. Their applications span petroleum production as well as transportation, waste storage, nuclear and bioengineering.

The effective physical properties of this class of materials are strongly dependent on the properties of their monolithic constituents and notably on their contrast **[1-4].** Over the last decades, effective medium theories **[5-7]** and variational models **[8-10]** were developed with the aim of predicting the behavior of porous media. An exhaustive and comprehensive review of all above theories is by given by **Pabst et al**. **[11]**

Mean-field theories and variational estimates yield predictions that agree well with available experimental data. On the other hand, such models predictions do not cover the entire range of porosity nor they can be used to predict the behavior of composites with more complex microstructures. **[4, 12]**

The aim of this study is to develop computer-assisted tools that allow complex microstructures to be tested and investigated. With this regard, rapid prototyping offers a promising technique for producing materials with controlled size, distribution and geometry of constituents and has so far been to study of the mechanical and transport properties of periodic prototyped foams and controlled scaffolds **[13-14]**. Here, we aim to exploit this technique for studying random heterogeneous porous materials. Specifically, focus of this paper is the prediction of their mechanical elastic properties of heterogeneous media. To this end, we combine experiments with numerical simulations. Porous microstructures with controlled and non-overlapping porosities are generated by means of a numerical algorithm. The latter generates a representative unit cell of a multiphase porous material using first order microstructure. The homogenized effective properties are then calculated numerically on the representative volume element (RVE) by using both kinematic uniform (KU-) and periodic boundary conditions (PBC). Finally, numerical results are compared with experimental measurements on 3D-printed porous specimens, whose microstructure is the same as that used for numerical simulations.

2. Algorithm for the generation of the controlled microstructure in heterogeneous materials

We use a random sequential addition (RSA) **[15-17]** algorithm to obtain a consecutive generation of inclusions in a unit cell. The inclusion, i.e. a non-overlapping object of quadric form, is randomly and sequentially placed into a unit-cell volume.

Input information for the algorithm is:

- The total volume fraction
- Number of pore's families.
- The reference number of particles, related to the characteristic size of the biggest family of pores.

For each family of porosity, the following features are assigned:

  - Characteristic size. This dimension is normalized with respect to the biggest characteristic size of the unit cell.
  - Aspect ratios of the pore.
  - Part of the total porosity.

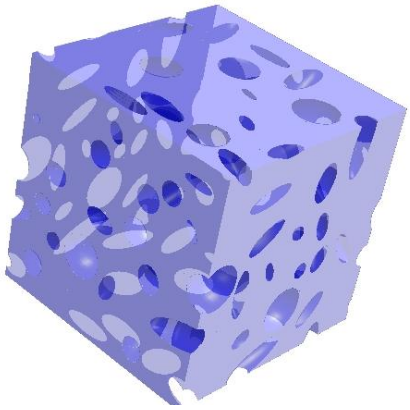

Figure 1: Generated microstructure with 20% porosity composed equally of 3 families of pores (spheres, prolates and oblates).

An example of a generated periodic unit cell with closed porosity uniformly distributed in the RVE is shown in figure 1. Note that in this study we focus on porous materials containing mono-dispersed spherical voids.

Once, the elementary unit cell is generated the RVE dimensions are identified. By definition, a RVE is the material volume which is assumed to be large relatively with respect to the size of the heterogeneities and whose behavior is independent on the boundary conditions (BCs). Its dimensions are therefore identified by comparing the response of microstructures with identical porosity under either periodic or uniform strain BCs. To this end, two porous microstructures with identical microstructural parameters are first generated. When constructing the unit cells, one is made periodic and periodic BCs are applied; uniform strain BCs are instead applied onto the as-generated microstructure. The commercial software *Abaqus* was used for the numerical analyses.

Figure 2 (left) shows the comparison between the effective Young's modulus (normalized with respect to the matrix modulus) obtained numerically when either periodic or uniform-strain BCs are applied onto microstructures featuring 10% porosity at increasing number of pores. The effective Young's modulus is obtained from the effective elastic stiffness tensor $\tilde{\mathbb{C}}$, the latter in turn obtained using the volume average tensors of the stress $\boldsymbol{\sigma}$ and strain $\boldsymbol{\varepsilon}$, respectively $\boldsymbol{\Sigma}$ and $\mathbf{E}$.

$$\langle \boldsymbol{\sigma}(\mathrm{x}) \rangle = \tilde{\mathbb{C}} : \langle \boldsymbol{\varepsilon}(\mathrm{x}) \rangle \qquad (1)$$

To compute the total stiffness tensor $\tilde{\mathbb{C}}$, uniaxial strain fields are applied and responses are superimposed. Note in passing that in the numerical analysis the matrix phase is assumed to be isotropic.

The ratio between the characteristic length D of the pore and that of the cell L (extrapolated from the RVE analysis) for microstructures containing increasing porosity is depicted in **figure 2 (right)**.

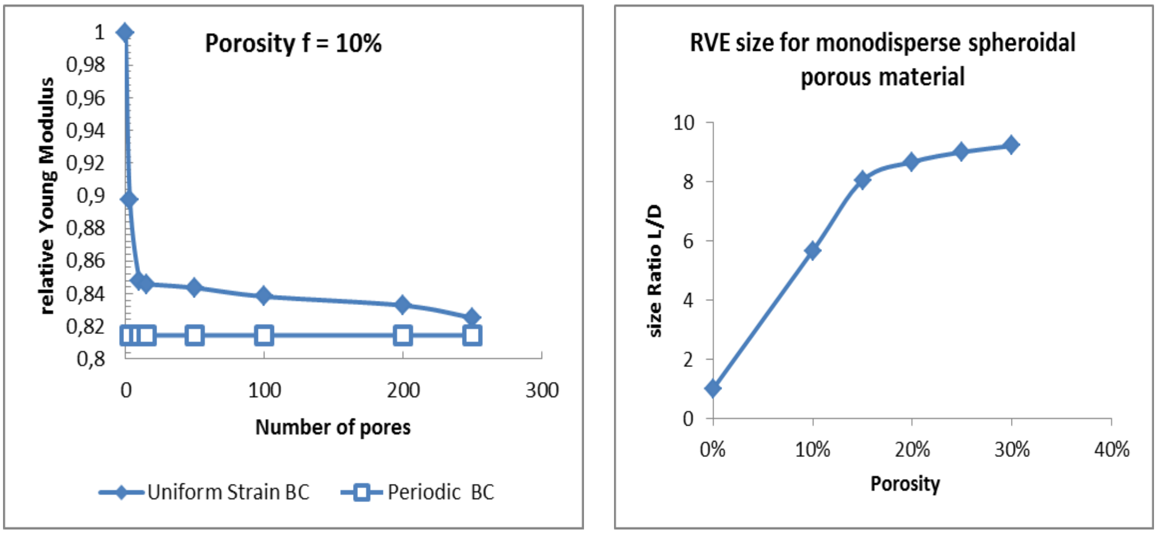

Figure 2: (left) RVE numerical analysis of a microstructure featuring 10% porosity. With an error of 5%, the number of reference pores is 75 which correspond to a ratio of size of 5,8.
(Right) Characteristic size ratio extrapolated from RVE analyses onto microstructures with increasing porosity.

3. Experimental results

Tensile testing was conducted onto 3D printed porous specimens. The computer-generated microstructures were first meshed using open-source software (Netgen **[18]**) and then exported into .stl (stereolithography) file format in order to be transferred to the 3D printer Startasys EDEN 260VS (France). A rubber-like material (trade-name Tango black) was used for printing the specimens and testing was conducting according to the standards (ASTM 632a **[19]**). Details of the printing Polyjet process are given by the manufacturer **[20]**. Note in passing that it was found experimentally that the printer resolution is 500um.

Prior to testing the porous microstructures, the bulk material properties were determined experimentally from tensile testing of 3D-printed solid specimens. The measured isotropic matrix material properties are E=3.9 MPa and v= 0.5.

Table 1 reports the parameters used for the printing the porous samples. These parameters are extrapolated from the RVE analysis (section 2).

Porosity(%)	**Pore number in the unit cell**	**Size Ratio for RVE**	**Size ratio in the unit cell**	**diameter of the pores(mm)**	**Experimental Young's Modulus (MPa)**
0	-	-	-	-	3.9
15	150	7	8.1	2.1	2.8
20	200	7.9	8.1	2.1	2.3
30	500	8.5	9.5	1.7	2.1

Table 1: Parameters used for printing the porous specimens

The comparison between the experimental measurement of the Young's modulus and numerical results is shown in Figure 3. Figure 3 indicates that there is a good agreement between the numerical predictions and the experimental data. Furthermore data lie within the Hashin-Shtrikman (HS) bounds**[21]**.

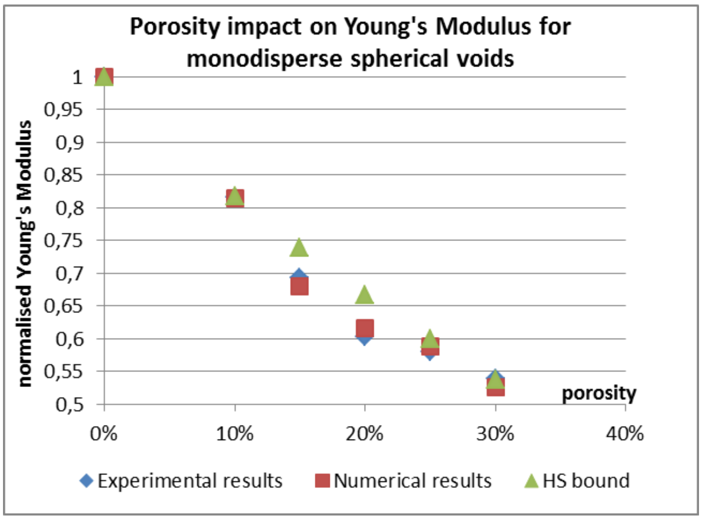

Figure 3: Comparison between the experimental measurements of the Young's modulus and the numerical results. Note in passing that (i) data are normalized with respect to the matrix modulus and (ii) data lie within the HS bounds.

4. Conclusion

A methodology for the determination of the effective properties of random heterogeneous materials has been introduced. Specifically, in this study we have focused on two phase porous material containing spherical voids and their effective properties have been determined both experimentally and numerically.

Three-dimensional porous structures, with non-overlapping porosity, were generated by means of a random sequential algorithm and numerical simulations where conducted on a representative volume element, whose size was first determined. Specimens were fabricated by 3D-printing of the computer-generated microstructures and tested under uniaxial loading. Results show a good agreement of the effective Young modulus.

Extensions of the algorithm are currently being made to the ellipsoidal randomly oriented voids as well as to unidirectional ellipsoidal voids.

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