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A cascade continuum micromechanics model for the effective elastic properties of porous materials

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ABSTRACT

The elastic properties of porous materials with a disordered pore structure are estimated using the mean-field *Eshelby* homogenization scheme together with the principle of recurrence to generate a cascade of effective microstructures as a function of the porosity and the cascade level *n*. Starting with the *Hashin–Shtrikman* upper bound for porous materials, the proposed cascade micromechanics model generates a hierarchy of micro-structures which evolve from an initial configuration of a porous material with spherical pores embedded within an elastic solid phase consistent with the *Mori–Tanaka* matrix inclusion morphology to a porous material characterized by a hierarchic distribution of spherical elastic grains. The model is explicit and allows for an easy computational implementation. It predicts physically consistent threshold porosities, characteristic for the specific morphology of the porous material under consideration, beyond which the material loses its stiffness. The validity of the cascade micromechanics model is evaluated against experimental data for various materials ranging from foam to ceramics with different pore structures.

1. Introduction

A large number of engineering, biological and geological materials such as ceramics, concrete, wood, bricks, rocks, polymers, biological tissues and bones are characterized by a heterogeneous porous micro-structure. Evidently, the pore-space is a fundamental micro-structural quantity which strongly determines the physical properties of the material such as the stiffness, strength, conductivity, permeability and diffusivity. Information about the dependence of these properties on the porosity (i.e. the ratio of the total volume of the pore-space to the total volume) and the topology of the pore-space is of fundamental scientific and engineering importance that has been intensively studied. In general, with increasing porosity, the macroscopic stiffness and conductivity decreases while the permeability and diffusivity increases. However, despite intensive research in the area of multiscale modeling, a unified quantitative relationship between the effective properties of porous materials and the relative size and the topology of the pore-space is still under investigation. The difficulties lie particularly in the different configurations of pore structure and adequate consideration of the pore space topology. Depending on the pore topology, different connectivity characteristics of the pore-space having the same total porosity may lead to different effective properties, which may vary considerably depending on the material type. Another challenge for homogenization models is the correct prediction of a percolation threshold (Broadbent and Hammersley, 1957) of the effective stiffness, i.e. a limit level of porosity, above which, due to the connectivity of the pore space and the missing inter-granular pathways, the material is no longer able to carry loads and therefore fails.

Voigt (1889) and Reuss (1929) proposed the first 'effective property' models through the rule of mixtures that reflect a parallel and a serial arrangement of the phases. The models provide the earliest bounds (Hill, 1963) on the effective elastic properties. For isotropic porous materials, the *Voigt* estimate is $k^V_{eff} = k_s\phi_s$ and $\mu^V_{eff} = \mu_s\phi_s$ and the *Reuss* estimate is $k^R_{eff} = \mu^R_{eff} = 0$. k_s, μ_s and ϕ_s are the bulk, shear modulus and the volume fraction of the solid phase. These are the widest possible bounds.

Assuming an isotropic distribution of the phases and macroscopic homogeneity, Hashin and Shtrikman (1963) derived improved bounds using a variational approach, given the volume fractions and the phase moduli. For two-phase porous materials, the bounds are obtained by exchanging the roles of the matrix and the inclusion in estimating the effective bulk and shear moduli. For the case of porous materials, the lower bound $k^{HS\downarrow}_{eff}$ (solid grains surrounded by a pore-space matrix) coincides with the *Reuss* estimate

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k^R_{eff} and the upper bound $k^{HS\uparrow}_{eff}$ improves the *Voigt* estimate k^V_{eff} such that for porous materials: $0 = k^R_{eff} = k^{HS\downarrow}_{eff} < k^{HS\uparrow}_{eff} < k^V_{eff}$.

Porous materials belong to the class of high-contrast matrix inclusion composites such that $\frac{k_p}{k_s} = 0$ as the bulk modulus of the pore $k_p = 0$. For this class of materials, the *Hashin–Shtrikman* (H–S) bounds cover a wide range of effective moduli, which maybe interpreted to be related to the large range of microstructure topologies, which varies from foam-like materials to ceramics. As a consequence, within these bounds, the connectivity of the phases and the corresponding percolation threshold strongly dictate the character of the effective property.

Since the 1960s, the *Eshelby* matrix-inclusion problem (Eshelby, 1957) (among others) has been applied in conjunction with volume averaging to estimate the effective properties of a wide range of heterogeneous porous materials (Dormieux and Kondo, 2005; Hellmich, 2005; Hill, 1965a; Lemarchand et al., 2003; Pichler et al., 2008, 2007). This methodology is referred to as continuum micromechanics (see, e.g. Hashin, 1983; Suquet, 1997; Zaoui, 2002 for an excellent overview). Within the framework of continuum micromechanics, according to the *dilute scheme*, the microstructure information is specified by a direct application of the *Eshelby* matrix-inclusion solution (Eshelby, 1957). As the name suggests, this scheme is applicable only for a low volume fraction of pores. However, the dilute scheme can be cumulatively applied in small increments, leading to the *differential scheme* (McLaughlin, 1977; Norris, 1985), which covers the complete range of porosities. One of the most widely applied micromechanics models is the *Mori–Tanaka scheme* (Benveniste, 1987; Mori and Tanaka, 1973), in which the far-field boundary condition used in the *dilute scheme* is modified to account for the interactions of the pores. In contrast to the aforementioned explicit schemes, the *self-consistent scheme* for porous materials (voids embedded in an elastic matrix) (Hill, 1965b) assumes that the phases are surrounded by the yet unknown effective medium, which leads to an implicit formulation. However, this scheme leads to physically meaningless solutions above a particular porosity (Budiansky, 1965; Hill, 1965b; Willis, 1977). While this particular porosity may be interpreted as a 'percolation threshold' (see Xia and Thorpe, 1988 for critical arguments against this interpretation), the explicit homogenization schemes such as the *Mori–Tanaka* scheme or the *differential* scheme, largely overestimate the effective elastic properties at high porosities and do not predict a threshold porosity, beyond which the material cannot sustain any loading (see Fig. A.15 in Appendix A). This holds both for spherical pores and an isotropic distribution of prolate (needle shaped) spheroidal pores in a solid elastic matrix. If an isotropic distribution of penny shaped pores is assumed, depending on the aspect ratio, a threshold can be predicted (see Fig. A.16 in Appendix A). However, while such a pore morphology is well suited for the representation of distributed cracks, it is not an appropriate morphology for the pore space of intact porous materials and therefore will not be considered in this paper. Thus, within the framework of continuum micromechanics, given the porosity of the material, the modeling of the pore structure requires the adequate choice of the homogenization scheme and the pore geometry.

As an alternative to using the framework of continuum micromechanics, numerical models maybe used to generate a discretized computational model of a representative elementary volume (REV) of porous materials to obtain effective elastic properties (see, e.g. Roberts and Garboczi, 2002; Wriggers and Moftah, 2006) from averaging. This approach allows direct incorporation of the complex pore space topology of a specific material, obtained, e.g. from CT measurements, into the model. Considering the considerable computational effort required for an adequate resolution of the pore space, currently computational homogenization methods only allow for the representation of a limited range of spatial scales.

In this paper, we propose a micromechanics model for the determination of effective elastic properties of porous materials, adopting the idea of self-similarity of hierarchical pore structures, which is based on a recursive scheme to obtain a cascade of matrix-inclusion problems. A similar concept was applied recently to the determination of effective diffusivities in porous materials (Timothy and Meschke, 2015). In addition to the porosity ϕ_p, the model is characterized by the cascade level n as a new order parameter to predict the effective elastic properties of porous materials. In contrast to power-law type models, which are generally based upon empirical fitting parameters, the cascade level n can be directly correlated with actual microstructure morphologies as the model is consistently formulated within the framework continuum micromechanics. For clarity and simplicity, we focus on spherical inclusions in the main part of the paper. For a discussion on the influence of the pore shape, also needle and penny shaped pore morphologies are addressed in Appendix A.

2. Continuum micromechanics of porous materials

In this subsection, a brief review of existing continuum micromechanics schemes is provided in order to provide a suitable introduction to the proposed model presented in Section 3. Within the framework of continuum micromechanics, the effective material properties of random porous materials can be determined, assuming the existence of a representative elementary volume (REV). The validity of the assumption of the REV is subject to satisfying the condition of scale separation. The characteristic length measures of the structure is assumed to be much larger than that of the REV at the 'macro-scale' which is again assumed to be much larger than the length scale of the heterogeneity (pores or grains) at the 'micro-scale'.

The total volume of the REV can be written as a sum of the volume of the pore-space V_p and the volume of the solid phase V_s:

$$V_{\text{REV}} = V_p + V_s. \tag{1}$$

A point in the domain Ω of the REV and on its boundary Γ is represented by the position vector $\mathbf{x}$. If a uniform macroscopic strain $\mathbf{E}$ is prescribed, the boundary conditions for the REV are given as (Hashin, 1983; Nemat-Nasser and Hori, 1999),

$$\mathbf{u}(\mathbf{x}) = \mathbf{x} \cdot \mathbf{E}, \quad \forall \mathbf{x} \in \Gamma \tag{2}$$

Denoting $\boldsymbol{\varepsilon}(\mathbf{x})$ as the local strain-field in the REV, which is subject to prescribed displacement boundary conditions (2), the volume averaged[1] strain in the porous REV is written in the form

$$\langle \boldsymbol{\varepsilon}(\mathbf{x}) \rangle_{\text{REV}} = \mathbf{E} = \phi_p \langle \boldsymbol{\varepsilon} \rangle_p + \phi_s \langle \boldsymbol{\varepsilon} \rangle_s. \tag{3}$$

$\phi_p = \frac{V_p}{V_{\text{REV}}}$ and $\phi_s = \frac{V_s}{V_{\text{REV}}}$ denote the volume fractions of the pore-space and the solid phase, respectively, such that, according to Eq. (1), $\phi_p + \phi_s = 1$. $\langle \boldsymbol{\varepsilon} \rangle_p$ is the average strain in the pore-space and $\langle \boldsymbol{\varepsilon} \rangle_s$ is the average strain in the solid phase. The following linear relationship is assumed between the strain $\mathbf{E}$ at the macro-level and the strain at the micro-level, i.e. in the pore space $\langle \boldsymbol{\varepsilon}_p \rangle$ and in the solid phase $\langle \boldsymbol{\varepsilon}_s \rangle$, respectively:

$$\langle \boldsymbol{\varepsilon} \rangle_s = \mathcal{A}_s : \mathbf{E}, \quad \text{and} \quad \langle \boldsymbol{\varepsilon} \rangle_p = \mathcal{A}_p : \mathbf{E}. \tag{4}$$

$\mathcal{A}_s$ and $\mathcal{A}_p$ are averaged fourth-order localization tensors of the solid phase and the pore phase. Substituting Eq. (4) into Eq. (3) provides the identity

$$\phi_p \mathcal{A}_p + \phi_s \mathcal{A}_s = \mathbf{I}. \tag{5}$$

[1] $\langle \cdot \rangle_i = \frac{1}{V_i} \int_{V_i} (\cdot) dV$