Computational Materials Science 97 (2015) 148–158

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Computational thermal conductivity in porous materials using homogenization techniques: Numerical and statistical approaches

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ARTICLE INFO

Article history:
Received 20 February 2014
Received in revised form 12 September 2014
Accepted 26 September 2014
Available online 6 November 2014

Keywords:
Numerical homogenization
Representative volume element
Porous materials
Effective thermal conductivity
Morphological analysis
Equivalent morphology concept

ABSTRACT

In this paper, the numerical homogenization technique and morphological analysis are used in order to compute the thermal conductivity in microscale of porous materials. The computational thermal homogenization is based on a 3D random material with spherical and ellipsoidal pores. Two types of microstructures are considered: microstructure 1 with random distribution of identical non overlapping pores and microstructure 2 with overlapping pores, based on the boolean model. The objective is to quantify the difference between these morphologies, in order to find some relationships between their morphological parameters and their macroscopic effective thermal conductivities. Periodic boundary conditions are applied on the representative volume element, *RVE*, of microstructures, for thermal modeling by finite element method. The covariance notion and integral range are introduced for morphological characterization. The deterministic *RVE* size is related with all microstructure parameters. The equivalent morphology concept for thermal conductivity is introduced after development of some relationships between morphological parameters.

1. Introduction

Heat transport through porous media is of great interest in chemical, mechanical, geological, environmental and petroleum applications. Recent applications of porous media arise in microelectronics for electronic packaging and bio-medical engineering. For these reasons, the determination of the effective linear thermal conductivity (ELTC) for various porous media is of great practical interest in the efficient design of industrial equipment. Generally, two techniques of homogenization are available in this topic, existing analytical estimates or computational numerical methods. The homogenization refers to the process of considering a statistically homogeneous representation of the heterogeneous material, called deterministic representative volume element (DRVE).

In the early years, analytical estimates for the effective thermal properties were developed and published in the case of porous media. For example, Progelhof et al. [1] give a review on methods for predicting the thermal conductivity of heterogeneous materials. Hashin and Shtrikman [2] proposed a more efficient framework for two-phase materials named HS bounds. The variational method is based on solving a problem of inclusions embedded in an infinite homogeneous matrix. For a further narrowing of the bounds, the third order bounds (3PB) of the thermal conductivity homogenization were developed in [3,4]. Some models or direct estimations are usually adopted to analyze and predict the thermal conductivity of porous media, including the two forms of Maxwell-Eucken models [5] and the effective medium theory model. For more explanations and mathematical expressions, see [6,7].

In the theory of effective thermal conductivity of mixtures, the analytical bounds are often used to validate and constrain thermal conductivity models, see [8]. For a high particles volume fraction and a high contrast between physical properties of phases, these bounds are too far apart to give a useful estimate of the effective properties. Therefore, it is necessary to develop numerical methods for predicting the effective thermal properties. The finite element method (FEM) is mainly used to perform a more reliable homogenization analysis.

Computational homogenization approach is widely utilized in the multiscale analysis of porous materials in order to obtain the effective properties. This approach has also been extended to the thermal field with a variety of applications. For real images of porous materials, Dorvaux et al. [9] and Grandjean et al. [10] have developed a method involving two and three-dimensional finite element calculations based on real micrographs of the ceramic materials and porous solid. The approach was tested on micrographs with pores ranging from 10% to 50%. For virtual images of

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http://dx.doi.org/10.1016/j.commatsci.2014.09.043
0927-0256/

ceramics, Qiang et al. [11] studied the numerical computational of the thermal conductivity with FEM. Bakker [12] investigated on the thermal conductivity of complex porosity by FEM. The effects of shape, orientation and distribution of the inclusion pores on the conductivity were studied. Bolot et al. [13] give the computation of heat transfer through a porous structure using numerical computation methods. It was also applied to thermal computations of random open-cell porous materials foams by Kanaun and Tkachenko [14], Wang and Pan [15], Laschet et al. [16] and Kanaun and Kochekseraï [17]. The homogenized effective thermal conductivities were compared there with various theoretical solutions and bounds. In the case of porous mullite material (is one of ceramic materials), Barea et al. [18] have studied the effective thermal conductivity with various particles volume fractions of pores. Tong et al. [19] have investigated the thermal conductivity of geological porous media by computational numerical simulations with various pores fraction. For three-dimensional (3D) case, the effect of different boundary conditions on ELTC of random microstructures (PBC: periodic boundary conditions, UGT: uniform gradient of temperature and UHF: uniform heat flux) is numerically analyzed and given in Kanit et al. [20].

Kachanov and Sevostianov [21] give the factors having strong and minor effects on overall conductive properties. They have shown for conductive properties, any isotropic mixture of diverse inhomogeneities is equivalent to a certain volume fraction of spheres. Florez et al. [22] have investigated on effective thermal conductivity of sintered porous media. They have shown that the geometry of the porous media solid matrix has an influence on the effective thermal conductivity.

To study the real effect of pores distribution and shape, it is necessary to develop another technique, based on microstructure morphology analysis. The morphology of porous media is characterized in order to obtain some morphological and thermal informations. Much progress has been made in characterizing the microstructure of statistically homogeneous two-phase random media via covariance and integral range. Such investigations are performed by Torquato [23], El Moumen et al. [24] and Paiboon et al. [25] for two-phase heterogeneous media with overlapping and non-overlapping spherical particles.

In this study, the computation of effective thermal conductivity in porous materials is proposed using numerical and statistical approaches. The first microstructure containing spherical pores without any contact between neighboring spherical pores and the second morphology with overlapping spherical pores. An equivalence between these microstructures is proposed. The numerical results are compared with available analytical solutions, such as HS bounds, 3PB, self consistent estimate (SC) of [26] and Maxwell-Eucken (ME) models.

After a general introduction, Section 2 outlines the microstructure generation and the subsequent finite element discretization. Section 3 presents numerical homogenization and details of results. Section 4 presents benefits of identifying and using statistical and morphological parameters and finally, in Section 5, these results are discussed.

2. The microstructure generation and the FE discretization

In this investigation, thermal numerical computations of porous materials, containing a random distribution of identical spherical or ellipsoidal pores are presented. Two types of microstructures are considered: microstructure 1 with non-overlapping spherical or ellipsoidal pores and microstructures 2 with overlapping pores, based on the boolean model of spheres. Fig. 1 illustrates the different positioning probabilities of two neighboring spherical pores in the microstructure of porous materials. Three different configurations controlled by a repulsion distance a were considered in this study, as shown in Fig. 1.

To generate the simulated microstructures, first pick points: $M_1, M_2, \ldots, M_i, \ldots, M_n$ in space at random locations, according to a Poisson process, see Fig. 2a. Next, construct pore i of each center M_i, with respecting a given repulsion distance a between neighboring pores in microstructure 1, and without respecting any repulsion distance for overlapping pores in microstructure 2. For ellipsoidal pores generation, the morphology of materials is completely defined by giving the center of each pore M_i, its principal radii a, b and c and its three orientation angles α_i, β_i and γ_i. These angles are also randomly chosen according to the Poisson process, see Fig. 2a. An example of 3D simulated microstructure with a random distribution of non-overlapping spherical and ellipsoidal pores in the space, obtained by Poisson process, is presented in Fig. 2b. As a result of microstructures generation, Fig. 3 shows examples of random implantation of overlapping and non-overlapping voids in porous materials based on the boolean model.

The regular finite element (FE) mesh is superimposed on the image of the porous microstructure using the so-called multiphase element technique. It should mention that this technique was developed by Lippmann [27] and extensively used by Kanit et al. [20] and El Moumen et al. [28] for homogenization of virtual and real 3D images. Indeed, an image of the microstructure is used to attribute the phase property to each integration point of a regular mesh, according to the color of the underlying voxel. Fig. 4 gives an example of the 3D microstructure and its FE structured and unstructured (free mesh) meshes. For numerical simulations, we prefer to use the structured meshes because the free mesh technique usually leads to larger numbers of elements, then more expensive in terms of computational cost. The considered elements are quadratic bricks of 20-nodes and 27-integration points per FE.

Both phases, matrix and pores, present a linear thermal conducting. The considered thermal conductivity for matrix phase is ranging from $\lambda_m = 0.3$ to 14.5 W/m K and for pores $\lambda_i = 0.024$ W/m K. The pore volume fraction f is also ranging from $f = 0.05$ to 0.5.

For mathematical morphology analysis, four cases are chosen:

- Case 1: $\lambda_m = 0.3$ W/m K and $\lambda_i = 0.024$ W/m K with contrast $c = \lambda_m/\lambda_i = 12.5$.
- Case 2: $\lambda_m = 0.5$ W/m K and $\lambda_i = 0.024$ W/m K with contrast $c = \lambda_m/\lambda_i = 20.8$.
- Case 3: $\lambda_m = 0.6$ W/m K and $\lambda_i = 0.024$ W/m K with contrast $c = \lambda_m/\lambda_i = 25$.
- Case 4: $\lambda_m = 14.5$ W/m K and $\lambda_i = 0.024$ W/m K with contrast $c = \lambda_m/\lambda_i = 604$.

3. Computational thermal simulations

3.1. Governing and constitutive equations

Generally, the 3D heat conduction is described by Fourier's law and given by:

$$\underline{q} = -\underline{\underline{\lambda}}\nabla T \tag{1}$$

where $\underline{q}$ is the thermal flux, $\underline{\underline{\lambda}}$ is the symmetric thermal conductivity tensor, T is the temperature and ∇T its gradient.

In elasticity problems, the boundary conditions are at the root of the energetic definition of effective elastic properties. Similar boundary conditions are prescribed for linear thermal conducting problems on the elementary porous microstructure volume V, see [29] for criterion and governing equations. In this study, we are concerned with random porous microstructures, and for this type of materials, the periodic boundary conditions converge faster in