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Effective elastic properties of periodic irregular open-cell foams

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ABSTRACT

This paper presents a micromechanical modeling for predicting the effective linear elastic properties of irregular open-cell foams using the periodic computational homogenization method. The tomography images are analyzed to obtain the morphological description of the irregular open-cell structure. An approach based on Voronoi diagram is used to generate realistic periodic foam structures with the morphological parameters. Hill's lemma computational homogenization approach is performed to predict the effective elastic properties. In this paper, we focus especially on the determination of the Representative Volume Element (RVE) and the importance of choosing the RVE parameters, i.e. the number of realizations and the volume of RVE, on the accuracy of models. The efficiencies of different approaches are discussed. Some recommendations and improvements are proposed.

1. Introduction

Thanks to the low solid volume fraction, high specific surface area and high specific strength, open-cell foams are very promising materials in various applications, such as in advanced thermal systems (Baillis and Coquard, 2008; Coquard et al., 2008), combustion systems (Gauthier et al., 2007; 2008), energy absorbers (Fischer, 2016; Jung et al., 2015), lightweight of transportations (Mukai et al., 1999), vibration damping (Yin and Rayess, 2014) and sandwich panels (Jing et al., 2016). This paper focuses on the computational effective elastic properties of open-cell foams from their microstructures.

In recent years, X-ray tomography has become a powerful non-destructive technique allowing to provide direct images of the heterogeneous materials at the relevant scale (Babin et al., 2007). The microstructure of cellular materials can be characterized (Maire et al., 2003) with the images. By means of tomography, Badiche et al. (2000) obtained Young's modulus, compression yield stress and tensile fracture stress of the open-cell nickel foams and compared them to the model of Gibson and Ashby (1997). Jang and Kyriakides (2009) characterized the microstructure of an open-cell aluminum alloy foam and monitored the evolution of crushing in compression experiments using computed X-ray tomography. Since the structures obtained by tomography are usually non-periodic and it is difficult to impose periodic boundary condition on non-periodic structure, Voronoi diagram is alternatively used to generate periodic regular or irregular foam models, so that periodic boundary condition could be imposed easily. Barbier et al. (2014) investigated the influence of the relative density and the irregularity of Voronoi closed-cell foam structures on their mechanical properties. Ye et al. (2015) considered regular tetrakaidecahedron Voronoi closed-cell foams and obtained a reasonable approximation of the shape of the loading surface using the Wang and Pan criterion for both yield surface and the failure surface. Open-cell foams have been generated by Voronoi diagram to calculate thermal conductivity (Baillis et al., 2017) and effective elastic properties (Zhu et al., 2017).

Hashin and Shtrikman (1962) and Hill (1963) proposed the homogenization theoretical principles to overcome the difficulties of modeling and computing caused by the huge dimension difference between structures and constituents. Subsequently, numerous numerical homogenization approaches (Fish and Belsky, 1995; Moulinec and Suquet, 1998; Kari et al., 2007; Fritzen et al., 2012; Geers and Yvonnet, 2016; Martnez-Ayuso et al., 2017; Brach et al., 2017; Rastkar et al., 2017) have been presented. The Finite Element Method (FEM) is widely used for heterogeneous materials (Feyel and Chaboche, 2000) and many approaches are based on it. By usual FEM, in order to obtain all the terms of the elasticity tensor, each model should be numerically solved 6 times with 6 independent elementary loadings (Kanit et al., 2003; Gatt et al., 2005; Moussaddy et al., 2013) with periodic boundary condition. A model has been proposed for heterogeneous media with periodic microstructure by formulating a variational statement with an asymptotic expansion of the energy functional (Yu and Tang, 2007a). This method, namely, the variational asymptotic method for unit cell homogenization (VAMUCH), has the ad-

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vantages that with only one finite element computation, effective properties could be determined without loadings.

The definition of the RVE is an essential part of the numerical homogenization (Moussaddy et al., 2013). The notion of the "theoretical RVE" reveals that a sample should be large enough to include a sufficient number of heterogeneities of the composite and to reflect the effective properties which are independent of boundary conditions (Hill, 1963; Drugan and Willis, 1996; Ostoja-Starzewski, 1998). From the practical standpoint, Gusev (1997) and Kanit et al. (2003) pointed out that the "numerical RVE" is defined as the smallest volume element which has the macroscopic properties. Gitman et al. (2007) listed some definitions of a RVE and a number of RVE determination criteria have been used before. Gusev (1997) proposed the first determination criterion to estimate the stability of the apparent properties with the increase of the heterogeneities. Kanit et al. (2003) presented that the number of random realizations of the volume element (with satisfactory confidence in the results) is also necessary to the RVE definition by algorithm. The effective properties would possibly be equal for small RVEs after a sufficient number of realizations and large RVEs after fewer realizations. Moussaddy et al. (2013) proposed a new RVE determination criterion, named averaging variations criterion, which is based on the statistical variations and applied it to analyze the fibrous media. Although several criteria have been reported (Kanit et al., 2003; Trias et al., 2006; Pelissou et al., 2009; Salmi et al., 2012; Ghossein and Lvesque, 2012) to determine RVE parameters for random composite models, there is no specific criterion for foam models.

In this work, the morphological description of real irregular open-cell foam is obtained by micro-computed tomography. With the tomographic data, the numerical periodic irregular models, which have same morphological features as the real foam, are generated using an approach based on Voronoi diagram. Hill's lemma computational homogenization approach (Zhu et al., 2017) is implemented to estimate the effective elastic properties of these models. The effective elastic stiffness matrix can be obtained with only one finite element calculation and without multiple loadings. Two RVE determination approaches (Moussaddy et al., 2013; Kanit et al., 2003) are performed and their efficiency and accuracy are analyzed. Based on these two approaches, specific methods are proposed to determine the RVE for the foam models.

2. Modeling of irregular open-cell structure

2.1. Morphological analysis of open-cell foam

A typical tomography slice of the irregular aluminum open-cell sample and the microstructure obtained by micro-computed tomography are presented in Fig. 1. The nominal porosity and the resolution of the sample are 94% and 22 µm per voxel, respectively.

2.1.1. Characterization of the geometry – covariance function

The covariance function (Matheron, 1975) and associated integral range are the basic statistical descriptors to characterize stationary and ergodic media. For a set X, the covariance function $C(X, \boldsymbol{h})$ denotes the probability for two points $\boldsymbol{x}$ and $\boldsymbol{x}+\boldsymbol{h}$ to belong to set X:

$$C(X, \boldsymbol{h}) = P\{\boldsymbol{x} \in X, \boldsymbol{x}+\boldsymbol{h} \in X\}, \tag{1}$$

where the vector $\boldsymbol{h}$ stands for the separation of the two points. Considering $h = \|\boldsymbol{h}\|$, for $h = 0$, $C(X, \boldsymbol{0})$ is the solid volume fraction of X. For $h \to +\infty$, the covariance shows an asymptotic value that equals to the square of the solid volume fraction. If the asymptotic value is reached before $h \to +\infty$, for example when $h = \mathcal{A}$, then the points with the separation larger than $\mathcal{A}$ are not correlated (Matheron, 1971), and the separation is the covariance range. Fig. 2 shows the covariance of the microstructure of the irregular open-cell sample in different directions. Covariance functions intersect the asymptotic value, and the covariance range is about 55 px. Since the covariance functions are similar in three directions, the microstructure can be considered geometrically isotropic.

2.1.2. Morphological parameters

In this paper, the superscript notations * and ^{b} represent homogenized and bulk properties, respectively. Based on the recent work (Zhu et al., 2017; Cunsolo et al., 2017), four morphological parameters are concerned to generate realistic numerical structures:

- Relative density, ρ^*/ρ^b, stands for the solid volume fraction.
- Coefficient of variation, C_V, shows the dispersion of cell size distribution of irregular structures and $C_V = \sigma_{d_c}/\overline{d_c}$, where σ_{d_c} denotes the standard deviation of cell diameter and $\overline{d_c}$ is the average equivalent cell diameter.
- Diameter ratio, t, controls the variation of the cross section area of a strut along the strut axis and $t = d_{min}/d_{max}$, where d_{min} and d_{max} are the minimum diameter and maximum diameter of the strut.
- Normalized curvature, k, describes the shape of cross section of strut. With variation of k, the shape of cross section varies from concave triangle ($-0.5 \leqslant k < 0$) to flat triangle ($k = 0$) to convex triangle($0 < k < 1$) and to circle ($k = 1$).

The tomographic data are analyzed with the free software iMorph (Brun et al., 2008) to extract the morphological parameters of the sample. The equivalent cell diameters present a Gaussian unimodal distribution with $\overline{d_c} = 2892$ µm and $C_V = 3.39\%$. Normalized curvature k and diameter ratio t have been proven to have significant influences on the effective elastic properties of open-cell foams (Zhu et al., 2017). Two analytical relationships among k, t and stereological measures are summarized in Cunsolo et al. (2017) as:

$$4S_{sur}/d_o^2 = 1.11k + 1.52, \tag{2}$$

$$\frac{d_o + d_i}{2d_{j,max}} = t^{\frac{2}{3}}, \tag{3}$$

where S_{sur} is the strut cross section surface, d_o denotes the strut cross section circumcircle diameter, d_i stands for the strut cross section incircle diameter and $d_{j,\,max}$ represents the strut junction maximum diameter (see Fig. 3). These geometrical measures are acquired by the cross section measurement function and the strut junctions measurement function available in iMorph. The morphological parameters of the irregular open-cell sample are $\left(\rho^*/\rho^b = 6.4\%; C_V = 3.4\%; k = 0.36; t = 0.34\right)$.

2.2. Generations of numerical structures

In order to numerically generate periodic irregular open-cell structures, a certain number of seeding points are generated first. With these points as the centers, the spheres with non-overlapping condition are generated by Random Sequential Absorption algorithm (Kraynik et al., 2003). The Voronoi diagram (Rycroft, 2009) partitions the given space into polyhedral regions for the seeding points, and then the generated structure is optimized by Surface Evolver (Brakke, 1992) to make it more realistic. The detailed description of the generation process can be found in Zhu et al. (2017) and Cunsolo et al. (2017). This generation method, including the use of Voronoi diagram and Surface Evolver post-processing, is inspired by Kraynik et al. (2003, 2004) for pure morphology and Jang et al. (2008) in study of mechanical properties. Additionally, in Cunsolo et al. (2017), this specific algorithm with respect to polyhedral cell geometry, has been validated by comparison with tomographic data, similar to Dillard et al. (2005). The