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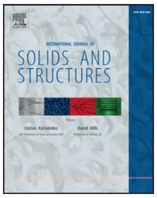

Comparison of full field and single pore approaches to homogenization of linearly elastic materials with pores of regular and irregular shapes

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ABSTRACT

Two approaches to predict the overall elastic properties of solids with regularly and irregularly shaped pores are compared. The first approach involves direct finite element simulations of periodic representative volume elements containing arrangements of pores. A simplified algorithm of collective rearrangement type is developed for generating microstructures with the desired density of randomly distributed pores of regular and irregular shapes. Homogeneity and isotropy (where appropriate) of the microstructures are confirmed by generating two-point statistics functions. The second approach utilizes Mori-Tanaka and Maxwell micromechanical models implemented via the cavity compliance contribution tensor (H-tensor) formalism. The effects of pore shape and matrix Poisson's ratio on compliance contribution parameters of different shapes are discussed. H-tensors of cubical, octahedral and tetrahedral pores for several values of matrix Poisson's ratio are published in explicit form for the first time. Good correspondence between the direct finite element simulations and micromechanical homogenization is observed for randomly oriented and parallel pores of the same shape, as well as mixtures of pores of various shapes up to 0.25 pore volume fractions.

1. Introduction

For many applications it is important to be able to determine how defects, and in particular pores, reduce the effective elastic properties of materials. There are several approaches to homogenization of porous solids including direct finite element analysis (FEA) simulations of representative volume elements (RVEs) of the material, micromechanical modeling schemes based on the solutions for individual defects, and establishment of variational bounds of Hashin-Shtrikman type, see, for example, discussion in Böhm et al. (2004). However, most of the existing literature is limited to the ellipsoidal shapes of defects since these shapes allow for convenient analytical solutions provided by Eshelby (Eshelby (1957), Eshelby (1959)). Meanwhile non-ellipsoidal pores are not only present in many natural and man-made materials (see examples in Sevostianov and Kachanov (2012)) but are also considered in design of additively manufactured end use components with deliberately engineered porosity (Choren et al. (2013)).

In this paper, we describe a numerical procedure to generate and analyze RVEs with non-intersecting pores of regular (ellipsoidal and polyhedral) and irregular shapes. We compare the results of direct FEA simulations with the predictions of two popular micromechanical schemes, Mori-Tanaka (Mori and Tanaka (1973), Benveniste (1987), Weng (1990)) and Maxwell (Maxwell (1873), McCartney and Kelly (2008), Sevostianov (2014)). The approach is illustrated by considering spherical, spheroidal, octahedral, cubical and irregular pore shapes. The latter was selected from microcomputed tomography (μCT) data obtained for a sample of 3D woven carbon/epoxy composite provided by Albany Engineered Composites (Rochester, NH USA). The pore shape is shown in Fig. 1.

Most of the published work on comparison of analytical micromechanical models with direct numerical simulations deals with the inhomogeneities of regular shapes such as spheres, spheroids and long fibers of circular cross-section. Segurado and Llorca (2002) numerically generated multiple RVEs with 30 spherical inhomogeneities utilizing the Random Sequential Adsorption (RSA) algorithm (Widom, 1966). They performed numerical simulations using FEA and compared their predictions of the effective elastic properties with several analytical homogenization models.

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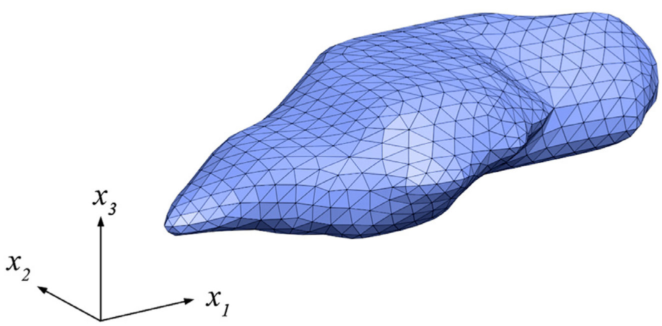

Fig. 1. Irregularly shaped pore obtained from μCT of carbon/epoxy composite sample.

The best correspondence was observed for the third order estimates of Torquato (1998). Later publications of that research group focused on nonlinear (elasto-plastic) behavior of composites with spherical and ellipsoidal inclusions, see for example González et al. (2004), Pierard et al. (2007).

Ghossein and Lévesque (2012, 2014) performed a comprehensive comparison of analytical and numerical homogenization results for random composites reinforced by spherical and spheroidal particles. They utilized an efficient, molecular dynamics based algorithm to generate random microstructures reaching significant particle volume fractions (up to volume fraction of 0.74 for monodisperse spheres, which is close to the theoretical limit of hexagonal close packing). The effective elastic properties were computed by applying a technique based on Fast Fourier Transforms (FFT) introduced in Moulinec and Suquet (1994) and Moulinec and Suquet (1998). The technique was shown to produce predictions very close to FEA – less than 1% difference for spherical particle reinforced composite with considered material properties. Note that recent findings by Gusev (2016a) indicate that the FFT-based method requires substantial computational resources for accurate predictions when composites with high material property contrasts are considered. In their two publications, Ghossein and Lévesque compared popular analytical homogenization schemes with numerical predictions for a wide range of material property contrasts, aspect ratios of the particles and their volume fraction. The authors limited their studies to microstructures with random orientation distribution of inhomogeneities of the same type, so the overall composite properties were isotropic.

El Moumen et al. (2015) addressed the influence of inhomogeneity shape on the effective bulk and shear moduli in the case of simulated microstructures containing randomly oriented non-overlapping particles. The authors focused on stiff particles of spherical and two spheroidal shapes (one oblate and one prolate) and used “multi-phase element” FEA to determine the effective elastic moduli of microstructures containing particles of the same shape. They compared their numerical results with the Hashin-Shtrikman bounds and Generalized Self Consistent scheme. In addition, they investigated the choice of the appropriate size of an RVE as a function of particle shape, material property contrast and volume fraction. The investigation was based on the statistical analysis involving microstructure covariograms and variations of effective properties between random realizations.

For composites with irregularly shaped inhomogeneities, several significant results are available in 2D. The solutions based on conformal mapping were utilized by Zimmerman (1986), Zimmerman (1991), Kachanov et al. (1994), Jasiuk et al. (1994), Tsukrov and Novak (2002), Ekneligoda and Zimmerman (2006), Ekneligoda and Zimmerman (2008), Zou et al. (2010), Mogilevskaya and Nikolskiy (2015). In 3D, Garboczi and Douglas (2012) presented a procedure to approximate bulk and shear elastic contribution parameters in the case of randomly oriented inhomogeneities shaped as blocks. The approximation is based on the solution for an ellipsoid with the additional correction factors derived by fitting analytical expressions to tabulated data from FEA results. Good correspondence between FEA results and the proposed approximation was found for a wide range of aspect ratios, matrix/inhomogeneity elastic contrasts and Poisson’s ratios.

Rasool and Böhm (2012) analyzed the effects of particle shape on the effective thermoelastic properties of composites reinforced with particles of spherical, cubical, tetrahedral and octahedral shapes. The authors performed FEA on five realizations of periodic structures with 20 particles of the same shape per RVE generated using a variation of RSA algorithm. Their results, however, were limited to a single stiffness contrast of 10 (particles stiffer than the matrix) and a single volume fraction value of 0.2. We compared our predictions obtained using Mori-Tanaka scheme based on the stiffness contribution tensor with the numerical results presented in Rasool and Böhm (2012) in a separate study (Böhm, personal communication) and obtained good correspondence (error within 1.2%). Recently, Böhm and Rasool (2016) extended the approach by considering elasto-plastic behavior of the matrix material.

Analytical micromechanical predictions of effective elastic properties are limited by the available elasticity solutions for an inclusion (portion of the matrix material with some prescribed eigenstrain) or inhomogeneity (portion of a different material inserted into the matrix material). In addition to the famous Eshelby solution for ellipsoidal inclusions (Eshelby (1957)), the analytical results for 3D inclusions and inhomogeneities of cubical (Faivre (1969), Chen and Young (1977)), cylindrical (Wu and Du (1995)), superspherical (Onaka (2001)), toroidal (Onaka et al. (2002)) and general polyhedral shapes (Rodin (1996), Nozaki and Taya (2001)) have been presented in the literature. However, not all of the solutions obtained for non-ellipsoidal shapes are convenient or appropriate for evaluation of contribution of the inhomogeneities to effective elastic properties. For materials with polyhedral inhomogeneities, the effective stiffness was predicted in Nozaki and Taya (2001); for convex superspherical inhomogeneities – in Hashemi et al. (2009). Both of these publications utilized analytical solutions in the framework of Mori-Tanaka scheme.

Numerical evaluation of contribution of individual inhomogeneity shapes also provides good basis for micromechanical modeling of effective properties. Sevostianov et al. (2008), Sevostianov and Giraud (2012) calculated contributions of superspherical pores; the accuracy of the calculations for concave superspherical pores was later improved by the authors in Chen et al. (2015). Drach et al. (2011), Drach et al. (2014b) used FEA to evaluate compliance contribution tensors for several irregular pore shapes relevant for carbon-carbon and 3D woven carbon-epoxy composites.

In this paper, we utilize the compliance contribution tensor formalism to produce analytical micromechanical predictions of effective elastic properties as discussed in Section 2. Our approach to numerical homogenization using FEA of RVEs with synthetically generated microstructures is presented in Section 3. The section also describes how we utilize two-point statistics functions to evaluate the homogeneity and isotropy of the generated microstructures. Predictions of the effective elastic properties for materials with pores of spherical, spheroidal, cubical, octahedral and an irregular shape are provided in Section 4. The results obtained by numerical modeling are compared with the estimates given by the Mori-Tanaka and Maxwell micromechanical models. Both parallel and random orientations of defects of the same shape are considered. The applicability of the method to mixtures of defects of different shapes is illustrated by modeling the material with