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Microstructure modeling of random composites with cylindrical inclusions having high volume fraction and broad aspect ratio distribution

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ABSTRACT

This paper presents a computational methodology for generating microstructure models of random composites with cylindrical or sphero-cylindrical inclusions having high volume fraction and broad aspect ratio distribution. The proposed methodology couples the random sequential adsorption (RSA) algorithm and dynamic finite element (FE) simulations. It uses RSA to generate sparse inclusion assemblies of low volume fraction and subsequently utilizes dynamic FE simulation for inclusion packing to achieve high volume fractions. The method can generate RVEs with volume fraction as high as 50% depending on the inclusion aspect ratio. Its capability is demonstrated by generating three distinct types of models with different inclusion characteristics which are further characterized in terms of homogeneity and isotropy. The results indicate that the proposed method is capable of generating models with low spatial variability of the filler orientation and volume fraction. The method can be used to generate input configurations for continuum and discrete representations of such random media.

1. Introduction

Macroscopic properties of inclusion-reinforced composites predominantly depend on the material microstructure. Particulate composites are usually random both in terms of the position of inclusions and their orientation (if non-spherical). While the mean filling volume fraction is defined, a non-uniform spatial distribution of inclusions may exist. Likewise, inclusions may have different morphologies and/or spatial orientation. Such variability has a rather small effect on the overall composite behavior, but has a large influence on the local field fluctuations, hence being of key importance for the prediction of damage nucleation and evolution.

A number of analytical and experimental methods have been developed in the literature to evaluate composite properties. Relevant reviews are presented in Refs. [1–3]. Many analytical models have been developed either based on Eshelby's strain tensor [4,5] or based on other micromechanics results [6,7]. Analytical methods were originally developed for unidirectional fiber reinforced composites and then modified to take into account random fiber orientation via tensor averaging [8] or classical lamination theory [9]. These models provide only bounds of the homogenized composite behavior because the microstructure of the composite is not represented in detail [10].

For random inclusion composites of high volume fraction, numerical modeling techniques, such as the finite element method (FEM), provide clear advantages. Finite element models represent microstructural details more effectively, and implicitly capture the field-mediated interaction of inclusions, which is usually represented only in the mean field sense in analytical models. Such simulations are performed using a statistically representative volume element (RVE) which is used to evaluate the average (homogenized) material properties. The RVE is the smallest volume over which a measurement can be made that yields a value representative of the composite behavior [11]. In order for a sample to be statistically representative, it should be large enough and should contain sufficient number of inclusions. The minimum size of the RVE is determined numerically by considering a sequence of models of increasing size.

Numerical generation of 3D RVEs for random inclusion composites (RIC) is inherently a challenging task [12]. For composites with periodic microstructure the periodic unit cell of the material can be chosen as RVE and the size of the model is dictated by the period of the microstructure. If no such internal characteristic length exists, the RVE size has to be determined numerically. To be statistically

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representative, such RVEs should contain sufficient information about the inclusion size, aspect ratio, orientation and spatial distribution. As the filler volume fraction and/or their aspect ratio increase, generating representative composite models becomes progressively more difficult. The prevalent method to generate such models is random sequential adsorption (RSA) [12–18]. In RSA inclusions are sequentially deposited in a box of desired size such that no two inclusions intersect and the distance between any two inclusions is always larger than a pre-defined threshold. The algorithm stops when the desired volume fraction is achieved or when no more inclusions can be added due to overlaps. Bohm et al. [16] implemented RSA to generate models of metal matrix composites with cylindrical or spheroidal fillers. They used 15 identical fibers with constant aspect ratio (AR) of 5 and achieved a volume fraction equal to 15%. Pan et al. [13] applied a modified RSA algorithm for a random fiber composite with fiber AR = 10 and achieved 13.5% volume fraction. Kari et al. [17] used a similar algorithm to generate models of randomly distributed short fiber and transversely randomly distributed short fiber composites with various volume fractions and aspect ratios.

The major issue with RSA-type methods is the existence of a geometrical jamming limit beyond which no additional inclusions can be added without overlap. This limits the volume fraction that can be reached [19]. Kari et al. [17] reported that the RSA algorithm cannot generate volume fractions larger than 25% for aspect ratios in the range $1 < AR \leqslant 10$. Several other authors also discussed the jamming limit, and the maximum achievable volume fraction has been similarly reported to be 20–25%, depending on the aspect ratio. To achieve higher volume fractions, Kari et al. [17] used different sizes of inclusions and deposited them in the descending order of their size. With this approach, they could achieve volume fractions up to 40%. However, this method is not applicable if all inclusions have the same aspect ratio. It also imposes limitations with respect to the distribution of filler size. Pan et al. [18] and Baliakanavar et al. [14] introduced local filler curvatures at points where sequentially deposited fillers overlap, in order to avoid their intersection and to reduce the algorithmic rejection rate at the same time. A volume fraction of about 35–45% has been reported for models with planar filler orientation. However, the local curvature introduced in the fillers leads to local stress concentration and the algorithm is inherently computation expensive because numerous filler intersection check-adjust loops must be executed.

This literature review indicates that currently available numerical tools lack the capability of generating microstructure models of RICs with high volume fraction at relatively low computational cost. In addition, it is important to develop numerical tools capable of generating models with realistic microstructural details. As mentioned above, a predefined constant gap is introduced between fillers in the RSA algorithm. This is arbitrary since in real materials the gap between two neighboring inclusions is entirely random. This limits the ability of the model to accurately predict the local stress state. Pan et al. [13] studied the effect of the gap size between two fillers embedded in a matrix. They found that the local stress concentration increases as the gap between fillers decreases and the effect becomes more pronounced at high volume fractions. In the present work we address these key issues.

This article presents a novel numerical method for generating RVEs of composites with randomly distributed inclusions. The proposed approach efficiently integrates the widely used RSA algorithm with dynamic FEM in order to generate composite models. Integration of dynamic FEM with RSA provides two distinct advantages. Firstly, it allows generate high volume fraction of inclusions. Secondly, inclusions can be packed more efficiently using this approach while satisfying the non-overlapping constraint. To overcome the jamming limit characteristic for RSA, we avoided generating inclusions in the actual composite domain in the first attempt. Rather we generate sparse and non-overlapping filler assemblies with low volume fraction in six pseudo-composite boxes surrounding the target box. Next, we perform a dynamic FE simulation based on transient dynamic FEM to push all inclusions into the target model box. Hence, all inclusions are packed simultaneously, which differs from iterative packing methods. Furthermore, a surface-to-surface based contact algorithm is used to prevent inclusion overlapping during packing. Contacts between inclusions are automatically detected and these are relocated accordingly to avoid intersection. The proposed method offers the following features that are superior to existing methods:

- It can generate composite models with volume fraction up to 50%, depending on the inclusion aspect ratio;
- Realistic microstructures can be produced by using specified distributions of inclusion geometries;
- It effectively uses the surface-to-surface based contact algorithm to prevent inclusion overlap instead of the computationally expensive iterative approach;
- The microstructure does not have any predefined gap between inclusions;
- The system is developed by integrating commercially available computer aided engineering tools, which facilitates the further extension and integration of this method with other systems.

The manuscript is organized as follows: a detailed description of different components of the proposed numerical system is presented in Section 2. Section 3 presents illustrative samples of the generated RVEs and a discussion on their geometrical features. In Section 4, we perform a microstructural characterization study by investigating randomness, homogeneity and isotropy of the generated RVEs.

2. Model generation framework

The proposed method for generating models with stochastic microstructure consists of three distinct components: (1) a sparse inclusion assembly generation step, (2) a packed inclusion assembly generation step, and (3) a step in which a CAD model of the problem domain is produced. The structure of this computational framework is illustrated in Fig. 1. The three steps are taken sequentially as suggested in the figure. This model generation concept is inspired from numerical optimization schemes developed in Refs. [20,21]. Details of the each system are discussed in the following sub-sections.

2.1. Sparse inclusion assembly generation

The objective of this step is to generate multiple sparse random inclusion assemblies with low volume fraction. These filler assemblies are generated using the RSA algorithm with an imposed minimum distance constraint between neighboring inclusions. We assume that inclusions have circular cross-section and model them as straight cylinders with a choice of aspect ratio and length. This assumption does not limit the applicability of the method to composites containing other types of inclusions. Inclusion axes are generated as line segments in a cubic box of size L, with random spatial position of their centers and random orientation. The dimension L coincides with that of the final, target model. For a fiber of length l, we first choose the position vector of one of its end points $\boldsymbol{P_0}$ as a random vector uniformly distributed on $[0, L]$ and two Euler angles θ and γ as shown in Fig. 2.

To ensure uniform random orientation over a unit sphere, two random variables uniformly distributed on [0, 1], u and v, are used and then the angles are calculated as [22]: