Effective properties of randomly oriented short and long fiber cases

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Abstract

In computational homogenization, the effective properties of random heterogeneous materials are obtained via the Deterministic Representative Volume Element, DRVE. By definition, the DRVE is the smallest volume of a heterogeneous media which is typical of the whole structure, which means its properties are independent of the effects of boundary conditions. Until now, it was considered that all heterogeneous materials with homogeneous inclusion distribution possessed a DRVE. The microstructure studied in this paper is a composite made up of randomly oriented short fibers(RSFC) and a computational homogenization is performed to investigate its effective properties. The area fraction is also varied to study its effect on the size of the DRVE. It appeared that at certain area fractions, the RSFC does not respect the convergence of the apparent properties calculated under different boundary conditions. This indicates that it does not adhere to the definition of the DRVE in the studied range of scale. The concerned area fraction is found to be around the percolation threshold. The present work consists primarily in investigating the causes of this problem by studying an extreme example of a percolating medium which is a composite made up of randomly oriented long fibers (RLFC). By identifying the contributing factors, the calculability of the DRVE of a random composite can be predicted by simple verification of the microstructure morphology.

Mots clefs: *Representative volume element; Numerical homogenization; Random media; Composite materials; Short fiber; Long fiber*

1. Introduction

Heterogeneous materials, unlike homogeneous ones, need to undergo a process called homogenization to find their effective properties. Nowadays, computational techniques are more widely used for the homogenization of heterogeneous materials. To achieve correct and precise calculations, the existence of a Representative Volume Element, RVE, is needed. An RVE has many definitions, but Hill [1] gave the classical definition which states that the RVE is a sample that is structurally typical of the whole microstructure, i.e. containing a sufficient number of heterogeneities for macroscopic properties to be independent of boundary conditions. Terada et al. [2] agreed that the RVE has to be as large as possible whileDrugan and Willis [3] stated that the RVE has to be the smallest volume possible where the apparent and effective properties converge and meet.

It is known that most heterogeneous materials possess an RVE, although the size may vary depending on the properties of each phase, the contrast, the type of inclusions and even the type of properties investigated: mechanical or thermal. Shahsavari and Picu [4]worked on bonded random fiber networks and stated that the RVE depends on fiber properties as well as fiber density. However, some porous materials like the 3D Poisson fibers of Dirrenberger et al.[5] may display an infinite integral range which contributes to a very large RVE or even the absence of an RVE. Either way, this means it is difficult to obtain correct results when carrying out the homogenization process. The same could be said for fibers with an infinite aspect ratio i.e. infinite fiber length.

In this paper, the computational homogenization method is first applied on a randomly oriented short fiber composite (RSFC) in 2D. It is widely known that short fiber composites possess a DRVE and this paper serves to verify its existence by varying the area fraction of the fibers. The search for the DRVE is then extended to a randomly oriented long fiber composite (RLFC). To distinguish it from the RSFC, the fibers in the RLFC are considered very long compared to their diameter, thus generating an infinite aspect ratio. The RLFC resembles the3D Poisson fibers studied by Dirrenberger et al.[5] and have shown that the mean apparent properties calculated from different boundary conditions do not converge even at large volume sizes. This investigation will verify if the non-convergent apparent properties are present in the RLFC. The goal of this study is to find the causes of the non-convergent properties by verifying its isotropy. Once they are identified, the *homogenizability* and the calculability of effective properties of any heterogeneous materials can be easily predicted.

2. Randomly Oriented Short Fiber Composites (RSFC)

2.1 Generation of the microstructure

Several samples of the RSFC is generated numerically with varying area fractions, A_f. Ten different RSFC are generated, starting with A_f= 0.11, A_f= 0.17, A_f= 0.23, A_f= 0.27, A_f= 0.32, A_f= 0.42, A_f= 0.51, A_f= 0.61, A_f= 0.71 and finally A_f= 0.81. It should be noted that A_f= 0.23 is the percolation threshold. These ten RSFC samples are illustrated in Fig. 1.

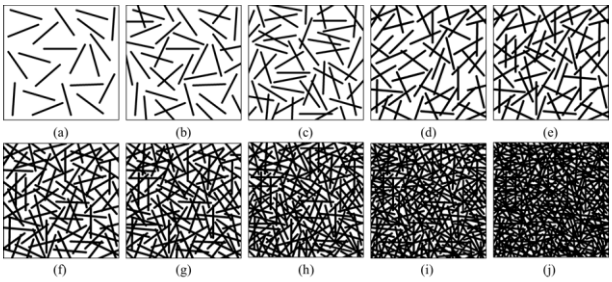

Fig. 1 Different microstructures of the RSFC arranged in ascending area fraction A_f

2.2 Computational homogenization technique

To carry out the homogenization of the RSFC, the finite elements (FE) calculations are performed using the methodology explained by Kanit et al.[6]. It consists in carrying out FE calculations in relation to the sample size. The homogenization method is carried out by selecting sample sizes *S* randomly from the macroscopic RLFC image, meshing it and performing FE calculations on it. This process is repeated until enough realizations *n* is achieved. To better understand this method, a visual representation of the different *S* and their distribution in the RSFC is illustrated in Fig. 2.

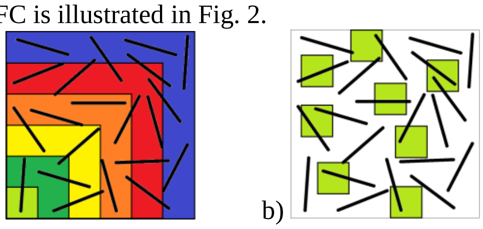

Fig. 2a) Different S used in the finite element calculations and (b) the random positions of the smallest S

2.2 Material properties and boundary conditions

For each individual *S*, two types of BCs will be applied. Kinematic Uniform Boundary Conditions (KUBC) and Periodic Boundary Conditions (PBC) are used in the calculation of elastic properties.

KUBC is described by imposing the displacement $\underline{u}$ at point $\underline{x}$ which belongs to the boundary ∂S :

$$\underline{u} = \underline{\underline{E}} \cdot \underline{x} \;\; \forall \underline{x} \in \partial S$$

where $\underline{\underline{E}}$ is a symmetrical second-order tensor independent of $\underline{x}$.

PBC has the same displacement field as KUBC but a periodic fluctuation $\underline{v}$ is added into the equation. The particularity with the PBC is that the fluctuation takes the same values at two homologous points on opposite edges of *S* :

$$\underline{u} = \underline{\underline{E}} \cdot \underline{x} + \underline{v} \;\; \forall \underline{x} \in \partial S$$

To determine the apparent mechanical properties, strain tensors $\underline{\underline{E}}$ are defined for the calculation of each elastic modulus. The calculations in this paper are strictly linear elastic with a plane strain hypothesis. For both KUBC and PBC, these strain tensors are applied in this manner for calculating the bulk and shear modulus:

$$\underline{\underline{E}}_k = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad ; \quad \underline{\underline{E}}_\mu = \begin{bmatrix} 0 & 1/2 \\ 1/2 & 0 \end{bmatrix}$$

The 2D apparent bulk modulus k_{app} and shear modulus μ_{app} are calculated using these equations:

$$k_{app} = trace\langle \underline{\underline{\sigma}} \rangle / 4 \quad ; \quad \mu_{app} = \langle \sigma_{12} \rangle$$

The properties such as the Young's modulus *Y*, the thermal conductivity λ and the Poisson's ratio ν attributed to each phase are detailed in Table 1. The contrast *c* is set to be $c_Y = Y_f / Y_m = 2000$. This high contrast is to ensure that the effect of the morphology on the behavior of the studied microstructures is more visible.

	Young's Modulus *Y* (GPa)	Poisson's ratio ν
Fiber	2000	0.3
Matrix	1	0.3

Table 1 Mechanical properties of the composite'sphases

2.4 Results

For simplification, only results of k_{app} is shown, knowing that other properties behave similarly. To verify the convergence of the properties precisely, the discrepancy errors of k_{app} from the KUBC and PBC are compared. Fig. 3 is an example ofhow the k_{app} of the RSFC sample with $A_f = 0.27$ do not converge with each other. In fact, the discrepancy error evolves with the A_f as shown in Fig. 4. The maximum discrepancy error seems to be around the percolation threshold. Furthermore, they tend to stay almost parallel from each other at larger *S* which lead to non-convergent properties. This means that the apparent properties are not effective. Without the convergence of the properties, the requirements of a DRVE which state that the properties should be independent of all boundary conditions are not satisfied.

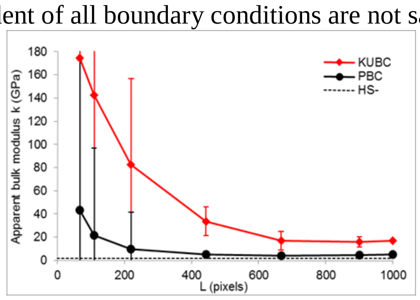

Fig. 3Mean apparent bulk modulus of the RSFC in relation to the sample size for $A_f = 0.27$

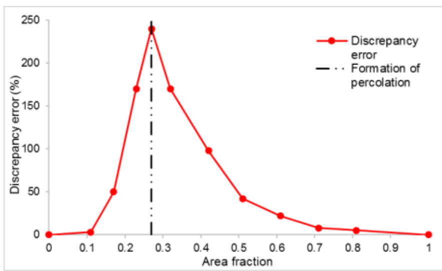

Fig. 4 Evolution of the discrepancy error in relation to the area fraction

3 Randomly Oriented Long Fiber Composites (RLFC)

3.1 Generation of the microstructure

The RLFC is made up of fibers with infinite aspect ratio and a random fiber orientation. In reality, the RLFC can be the equivalent of long fiber non-woven materials studied by Demirci et al. [7]. The morphology of the RLFC is made of a Boolean model which is widely used for generating stochastic models. The idea is to embed points randomly in a 2D plane according to a Poisson process and generating straight lines from these points at random orientations. Fig.5 shows the generated microstructure of the RLFC. The same properties and homogenization technique are applied in this section.

Fig. 5 Microstructure of the RLFC with A_f = 0.51

3.2 Results

It is seen that the apparent properties resulting from both the KUBC and PBC are far apart from each other even with larger *S*, as it is with the case of the lowly percolated RSFC. This behavior is also observed by Dirrenberger et al.[5] in 3D Poisson fibers. This means the apparent properties are not expected to converge and thus are not effective.For the RSFC, one factor that caused the non-convergent properties is the anisotropy created by a chain of fibers. The RLFC, however, has percolating fibers directed in every direction so, in principle, the bias in the mechanical response should have already disappeared. To verify if there really is an anisotropic response in the RLFC, a study on its elastic moduli tensor is done.

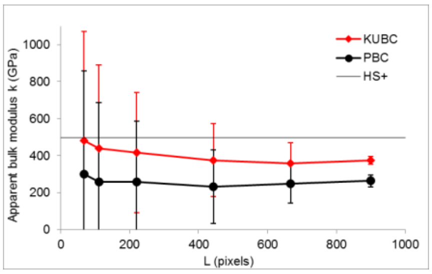

Fig. 6 Mean apparent bulk modulus of the RLFC in relation to the sample size

3.3 Elastic moduli tensor

To verify the isotropy of the microstructure, it is imperative to calculate the stiffness matrix $\underset{\sim}{C}$ .The full apparent stiffness matrix $\underset{\sim}{C}^{app}$ for both boundary conditions along with the intervals of confidence are presented below:

$$\underset{\sim}{C}^{app}_{KUBC} = \begin{bmatrix} 672\pm48 & 188\pm18 & 10\pm15 \\ 188\pm18 & 424\pm60 & 22\pm14 \\ 10\pm15 & 22\pm14 & 185\pm15 \end{bmatrix} \text{(GPa)}$$

$$\underset{\sim}{C}^{app}_{PBC} = \begin{bmatrix} 515\pm34 & 113\pm12 & 8\pm12 \\ 113\pm12 & 283\pm80 & 21\pm12 \\ 8\pm12 & 21\pm12 & 132\pm10 \end{bmatrix} \text{(GPa)}$$

The anisotropy index *a* calculated from both $\underset{\sim}{C}^{app}$ shows that $a_{KUBC} = 0.76$ and $a_{PBC} = 0.66$, which are quite far from isotropy (*a* = 1.0). This makes the RLFC anisotropic. Demirci et al. [7] studied nonwoven fibers which cross from one edge to the other and are oriented randomly like the RLFCand have found that the fibers are very direction-dependent.

However, it is uncertain that these observations and conclusions remain valid for larger scales. Even without convergence of mean properties, Dirrenberger et al.[5]estimated that the RVE of 3D Poisson fibers exists but is very large. This may also be true for the RLFC, where a larger scale would result in a homogeneous distribution of fibers and an isotropic behavior. What is clear is that in the scale of this study, the DRVE of the percolating RSFC and the RLFC cannot be calculated without the existence of effective properties.

4. Conclusion

Indeed, there are heterogeneous materials with homogeneous distribution of inclusions which do not possess converging effective properties. In this paper, we have found the two contributing morphological features; random infinite fibers and percolating fibers.Further studies on these "problematic" microstructures need to be carried out to better understand their behavior, especially to verify the convergence of the mean apparent properties at higher range of scales. Nevertheless, it is certain that no convergence is observed in the scale of this study.

References

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