Influence of morphological parameters of a 2D random short fibre composite on its effective elastic properties

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Abstract :

The paper deals with the assessment of the influence of morphological parameters of a 2D random short fibre composite on its effective elastic properties. A double-scale 2D finite element approach is used and periodic representative volume elements are generated according to the model with an norder approximate geometry. This one is a recent and powerful tool to generate meshes in the context of complex microstructures such as random fibre composites. Impact of three morphological features namely, aspect ratio, tortuosity of fibres and width of the interphase area, is investigated. Numerical results are provided for several contrasts of properties and volume fractions of fibres.

Résumé :

La contribution porte sur l'étude de l'influence des paramètres morphologiques d'un composite 2D à renfort fibre courte sur ses propriétés élastiques effectives. Une approche éléments finis et doubleéchelle 2D est considérée et nous générons des volumes élémentaires représentatifs du matériau selon une stratégie de maillage dite d'approximation d'ordre n. Il s'agit d'un outil efficace mis au point récemment afin de générer des maillages sur des microstructures complexes. Dans le présent papier, nous focalisons notre étude sur l'impact de trois paramètres, à savoir, l'élancement et la tortuosité des fibres ainsi que la largeur de la zone d'interphase. Des résultats numériques sont fournis pour différents contrastes de propriétés et fractions surfaciques d'hétérogénéités.

$Mots\ clefs:$ computational solid mechanics; short fibre composites; RVE

1 Introduction

For several decades short fibre composites have been manufactured and used for industrial purposes. Their low cost of production associated to their excellent strength-to-weight ratio have led to numerous applications in many fields like aerospace, automotive engineering, and competitive sport. For examples, fibreglass is massively produced for building hulls in marine industry and carbon-fibre-reinforced composites are used for retrofitting old structures in civil engineering. The main issue is to assess their intrinsic mechanical properties in order to evaluate their ability to replace one-phase materials. Experimental measurements are sometimes difficult and costly to set up for this purpose. That is why analytical models are very useful for estimating effective properties. Mori-Tanaka micromechanics model [9] and self-consistent estimates [4] are classical tools for predicting elastic coefficients of two-phase heterogeneous media. However, accurate predictions of the mechanical response are difficult to obtain since this one strongly depends on several parameters such as orientation, shape and aspect ratio of heterogeneities. Thus, numerous micromechanics models have been proposed during the last



FIG. 1 – Parametrisation of the tortuosity of a fibre

decades for improving the accuracy of estimates, among which, the general self-consistent scheme [1] and the third-order approximation [13].

However, the range of validity of a micromechanics model is always restricted. Thus, there is no model for complex-shaped heterogeneities, for example tortuous fibres, for which no Eshelby's tensor is available. In this context, a numerical modelling is more convenient to evaluate effective properties. The basic idea consists in generating a Representative Volume Element (RVE) of the material either by a Random Sequential Adsorption (RSA) [12] for which distance constraints prevent the overlap between two or more heterogeneities, or a fully Monte-Carlo (MC) process [3]. Effective elastic properties are generally evaluated either with the help of a Fast Fourier Transformation [10], or more classically, by Finite Element (FE) analysis [6]. Unfortunately, in the context of random heterogeneous media, a FE approach is difficult to set up since the mesh generation is thwarted by several drawbacks related to the complex structure of the network of heterogeneities. Hence, a modelling of such a microstructure is often basic and unrealistic. However, the recent development of the model with an n-order approximate geometry [7] which is based on a grid approximation, has opened prospects for the generation of complex microstructures. In the present work, a FE approach using this concept is considered in order to assess elastic coefficients of a 2D random short fibre composite for which the microstructure is complex and strongly entangled. Influence of three morphological parameters namely, aspect ratio, tortuosity of fibres and width of the interphase area, is investigated.

2 Numerical modelling

2.1 Morphological parameters

2D microstructures are generated according to a set of random morphological parameters describing the complex geometry of a random fibre composite. Each parameter is either randomly drawn according to a given distribution law such as, for example, the Gaussian and uniform ones, or fixed. On the one hand, both centroid spatial location and orientation of each heterogeneity are randomly drawn. One must keep in mind that we assume no distance constraint between two or more fibres so that the process can be seen as a MC one. Thus, all distribution laws are unbiased, and the overlap between two or more fibres is possible. On the other hand, other parameters are set at given values in order to be investigated in a deterministic way,

- the **aspect ratio** a_r of fibres which is the ratio between the length l and the diameter d of each heterogeneity,
- the parameter of **tortuosity** of fibres which describes the level of non-straightness of a heterogeneity. This one is defined by a maximum angle θ_m which has to be respected in the generation of a fibre in the same way as [2]. Fig. 1 illustrates how one set up a tortuous fibre. The process consists in building the reinforcement point by point starting from its centroid G. Thus, each new point P_{i+1} is obtained from its predecessors P_i and P_{i-1} considering the distance between two consecutive nodes l_i , and an angle θ_i which is uniformly drawn between $-\theta_m$ and θ_m . l_i is chosen constant and sufficiently small to ensure the smoothness of the heterogeneity.
- the width w_{int} of the **interphase area**. This one is an area surrounding each reinforcement where the properties of the matrix are disrupted due to the presence of the heterogeneity. One must take care of not confusing interphase with interface which designates the boundary between soft and hard phases. In the present work, no decohesion is taken into account and perfect bondings are supposed.



FIG. 2 – RVE obtained according to the model with a 2-order approximate geometry (100-by-100 coarse grid)

2.2 RVE

The investigation of the dimensions of the RVE is a key issue from which representativeness, efficiency and validity of the numerical modelling strongly depend [5]. The size of an RVE is defined as s, the scale ratio between its width and the average length of each heterogeneity. s must be greater than a critical scale ratio s_r to check out the representativeness of a unit cell and avoid a bias introduced by the boundary conditions. Its assessment is realised according to the process described by [5] which leads to a compromise between accuracy of results and low cost of calculation. In the present work, an RVE is generated from the set of random and deterministic parameters described in 2.1. In addition, a specific treatment is performed to ensure the periodicity of the cell. Its principle consists in duplicating and translating the fibres intersecting the boundaries of the unit cell.

2.3 Mesh generation

A reliable, efficient and automated mesh generation of overlapping random heterogeneous media is particularly difficult to set up in a classical approach for which the mesh is directly generated from the boundaries of the network of fibres. The voxel-based FE approach [8] circumvents the drawbacks relative to the mesh generation. This one consists of approximating the boundaries of the network of fibres according to a grid of pixels in 2D or voxels in 3D. The concept is very suitable for a reliable and automated mesh generation but is poorly efficient. The last point is drastically improved in the context of a strongly entangled microstructure when using the model with an n-order approximate geometry [7]. This one is based on a 2-step mesh generation. First, one has to generate a grid of coarse elements the size of which is typically equal or greater than the diameter of fibres. Second, an adaptive mesh refinement (AMR) is performed in order to locally refine the boundaries of each heterogeneity according to an n-order parameter. This one is defined as the ratio between the diameter of fibres and the size of the smallest voxel, expressed in logarithm in base 2. Thus, a Delaunay triangulation constrained to the approximate boundaries enables a reliable and automated mesh generation. In addition, it was exhibited [7] that the n-order strategy leads to a tremendous reduction of the calculation cost in comparison with a classical approach without AMR. Fig. 2 illustrates an RVE obtained according to the model with a 2-order approximate geometry before meshing. The red phase (1) corresponds to the reinforcement, the blue one (2) corresponds to the interphase area and the yellow one (3) corresponds to the matrix phase. Morphological parameters are as follows, w_{int} is set at d/4, a_r is set at 20, θ_m is set at 40° and s is set at 5. The number of heterogeneities is set at 100.

3 Influence of morphological parameters

An investigation of a set of morphological parameters, namely the aspect ratio, the tortuosity and the width of the interphase is set up under the following hypotheses. First, effective elastic properties are evaluated according to the asymptotic process described by [5]. This one consists of generating a complete sample of RVEs for which elastic coefficients are assessed by a homogenisation technique namely, in the present work, the double-scale approach [11]. Effective properties are then obtained from averaging the scope of results. Second, we consider networks of randomly distributed and oriented fibres. Each one follows an isotropic transverse behaviour law and the soft phase is isotropic. Y_l^f, Y_t^f, μ^f and κ^f designate longitudinal and transverse Young's, shear and bulk moduli of each fibre respectively. Y^m, μ^m and κ^m are Young's, shear and bulk moduli of the matrix respectively. Poisson's ratios are equal to 0.25 and 0.35 for hard and soft phases respectively. In addition, we set $Y_l^f = 2Y_t^f$. κ^* is the normalised effective planar bulk modulus which is estimated as follows,

$$\kappa^* = \frac{1}{4\kappa^m} \sum_{\alpha,\beta \le 2} C_{\alpha\alpha\beta\beta} \tag{1}$$

where $C_{\alpha\beta\gamma\delta}$ $(\alpha, \beta, \gamma, \delta \in \{1, 2\}^4)$ is the effective stiffness tensor. In addition, interphase area is supposed isotropic with shear and Young's moduli equal to 0.5 times the ones of the soft phase. The contrast of properties c_r between hard and soft phases is defined as follows,

$$c_r = \frac{Y_l^f}{Y^m} = \frac{\mu^f}{\mu^m} \tag{2}$$

Finally, meshed are built according to the model with a 2-order approximate geometry, and the size of RVE s is set at 5 according to previous investigations [7].

3.1 Aspect ratio



FIG. 3 – Influence of the aspect ratio on the normalised effective bulk modulus (a) $c_r = 10$ (b) $c_r = 50$

First, a study is realised for a range of aspect ratios a_r between 5 and 50. θ_m is equal to 20 and w_{int} is equal to d/4. Several volume fractions of fibres are considered between 5 and 25 %. Fig. 3 (a) illustrates the influence of the aspect ratio on the normalised effective bulk modulus κ^* for a contrast of properties set at 10. One can notice that the greater the aspect ratio is the greater the bulk modulus is whatever the load rate is. Thus, κ^* varies from 1.2690 to 1.4529, for a volume fraction of fibres of 25 %, when the aspect ratio goes from 5 to 50. Results are similar with higher values in the case of a high contrast of properties (Fig. 3 (b), $c_r = 50$) for which κ^* varies from 1.5171 to 2.4033 for a volume fraction of fibres of 25 %. One can notice that the saturation is almost reached when c_r is equal to 10 while this one is barely noticeable for a high-contrast composite. This result is related to end effects which much more impact the mechanical response of the material when the contrast is important.



FIG. 4 – Influence of the maximum angle on the normalised effective bulk modulus (a) $c_r = 10$ (b) $c_r = 50$

3.2 Tortuosity

Second, the influence of the tortuosity of fibres is examined. Maximum angle θ_m is set at several values between 0 for which fibres are straight and 40° for which fibres are strongly tortuous. a_r is set at 20, w_{int} is set at d/4 and several volume fractions of fibres are considered between 5 and 25 %. Fig. 4 (a) illustrates the influence of the tortuosity of fibres on κ^* for c_r set at 10. On the one hand, results highlight a slight negative impact of the tortuosity for a low contrast of properties. Thus, κ^* varies from 1.4226 to 1.3767 when θ_m goes from 0° to 40° and the volume fraction of fibres is 25 %. In addition, κ^* goes from 1.10587 to 1.0676 when θ_m varies from 0° to 40° and the volume fraction of fibres is 5 %. On the other hand, discrepancies are greater when the contrast of properties is higher (Fig. 4 (b), $c_r = 50$). Thus, κ^* varies from 2.3322 to 2.0730 when θ_m goes from 0° to 40° and the volume fraction of fibres is 25 %. However, the influence of the tortuosity is still slight when the load rate is low. Indeed, κ^* varies from 1.1630 to 1.1337 when θ_m goes from 0° to 40°, the volume fraction of fibres is 5 % and c_r is 50.

3.3 Width of the interphase area



FIG. 5 – Influence of the width of the interphase area on the normalised effective bulk modulus (a) $c_r = 10$ (b) $c_r = 50$

Finally, the width of the interphase area is investigated. This one is chosen between 0 for which there

is no interphase area and 0.75 times the diameter of fibres. One must keep in mind that a_r is set at 20, θ_m is set at 20 and several volume fractions of fibres are considered between 5 and 25 %. Fig. 5 (a) shows the influence of the width of the interphase area on κ^* for a contrast of properties set at 10. The wider the interphase area is the lower the properties are whatever the load rate of heterogeneities is, which is consistent with the fact that the interphase area is less stiff than the soft phase. Thus, κ^* varies from 1.5450 to 1.2240 when the volume fraction of reinforcements is 25 % and w_{int} varies from 0 and 0.75*d*. The same one goes from 1.0907 to 1.0156 when the volume fraction of reinforcements is 5 %. In addition, Fig. 5 (b) depicts the influence of w_{int} on κ^* for a contrast of properties set at 50. Results are quite similar to the previous ones. Thus, κ^* varies from 2.4487 to 1.9358 when the volume fraction of fibres is 25 %.

4 Conclusions

An investigation of the influence of morphological parameters of a 2D random short fibre composite on its effective elastic properties has been set up. Conclusions are as follows. First, results confirm the benefit of using long fibres rather than short ones. Second, non-straight fibres slightly affect the mechanical response, expecially when both volume fraction of fibres and contrast are high. Finally, the interphase area drastically reduces the reinforcement of the material whatever the contrast of properties is.

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