A MORPHOLOGICAL INDICATOR FOR THE DESCRIPTION OF THE SHORT-FIBER POSITION EFFECT ON THE BEHAVIOR OF A PERIODIC RVE

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Abstract
This paper introduces an identification method of a microstructural indicator in a unidirectional short-fiber reinforced composite. Following a design of experiments (DOE), virtual microstructures were generated by finite elements in a previous approach for the determination of a RVE of the material. A global indicator of the behavior was first defined and allowed sorting the volumes compared to a convergence behavior. Those results showed that only one volume was perfectly reaching the convergence behavior among ten generated ones. In order to understand this result, a microstructural indicator, based on the first neighbor distance of the fibers in the microstructures, was defined to understand the impact of their morphology on their global elastic behavior. The results showed that this microstructural indicator could allow a pertinent shortlist of possible RVE and avoid several finite element computations for the acquisition of accurate microstructures in terms of behavioral performances.

1. Introduction

Today, a greater respect for the environment is at the heart of industrial concerns and is added to performance and cost targets. Lightening and optimizing the structures is one of the levers to address this goal. The use of short fiber reinforced thermoplastic composites offers interesting possibilities to replace traditional metal parts while allowing complex and optimized geometries. The modeling of short-fiber reinforced thermoplastic parts requires a detailed comprehension of their behavior, which highly depends on their microstructure. However, the available computing power does not often allow such a detailed modeling of the entire microstructure [1]. The notion of Representative Volume Element (RVE), introduced by Hill [2] and improved in many works [3], [4], [5] is often used to deal with such composite materials. The work of Kanit *& al.* [6] discusses the principle of RVE in the case of randomly reinforced materials where there is no repeatable pattern. Thus, a statistical component had to be taken into account for the determination of a RVE; this volume must be called a Statistically Representative Volume Element (SRVE).

The determination of the SRVE is a first step towards the modeling of a short fiber reinforced composite material. Although the manufacturing process of these materials implies a misalignment of the fibers through its thickness [7], this work focuses on a smaller scale where unidirectional reinforcement orientations might be considered. This consideration allows to free ourselves from the use of orientation tensors, which are approximations needed for higher scale representations.

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Furthermore, some modeling strategies are already available to deal with fiber orientations and many of them are based on an average of the unidirectional properties over all possible directions, weighted by an orientation distribution function [7]. Those strategies could be associated to the modeling presented in this paper.

A full field computing chain for the volume generation was conducted and leaded to the creation of 180 different microstructures in a previous work. A global indicator based on the elastic behavior of the microstructures allowed their ranking in terms of performances [8]. Those results are briefly presented at the beginning of this paper. The main goal of this work is thus to provide a strategy to achieve the most efficient numerical SRVE based on a microstructural indicator. The main subject of this paper is an original method to understand the influence of the morphological dispersion in a class of microstructures on their stiffness behavior. This method is an extension of the known work in 2D [8], [9] and introduces a microstructural indicator based on the first neighbor distance of the fibers in a specific microstructure.

2. Previous work

This part deals with the presentation of the earlier work done on the volume generation, which is not detailed in this paper. The purpose of this work was to generate several microstructures of different sizes, which were computed in order to estimate a full field homogenization of their elastic behavior. The choice of a finite element modeling was preferred to a FFT one because it offers more possibilities in non-linear computations. The DOE of the generated volumes and the full field computing chain by finite elements are presented. The determination of the SRVE thanks to a global performance indicator is briefly explained.

2.1. DOE and volume generation process

The presented method is generic and applicable to all short-fiber reinforced composite materials. In this work, the matrix was considered as elastic, isotropic and reinforced by 19% in volume by transversally isotropic short fibers. The dimensions of the fibers are around 7 micrometers in diameter (d_f) and around 150 micrometers in length (L_f). According to these data, a generation tree was defined for the generation of the 3D volumes (
Figure **1**).

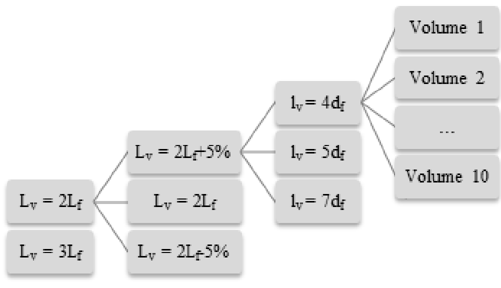

Figure 1. Microstructure generation tree

The 3D volumes are parallelepipeds whose length is L_v and whose thickness and width are equal and called l_v. The presented generation tree allows dispersion in terms of fiber positioning in the space of each volume. Ten specimens of each volume were generated in order to introduce a statistical component in this study. A total of 180 3D microstructures were generated. Each group of volumes of the same size was called a “class”. The main hypothesis of the 3D generation was about the periodicity of the volumes. Indeed, Forest [11] showed that the behavior of periodic volumes faster reaches a convergence behavior, as the volume size increases, than non-periodic volumes. In order to take benefits from this observation, the unidirectional volumes have been modelled as periodic ones.

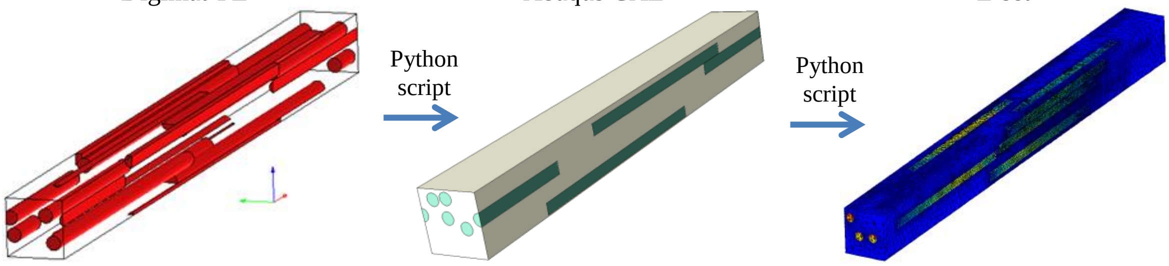

Figure 2. Full field computing chain

Three different software were used for the generation of the 3D finite element microstructures. Digimat FE, from the Digimat software suite [12], has been used for the geometric generation of the 3D microstructures. Via a Python script, the microstructures were regenerated in Abaqus CAE [13], where an adaptive meshing was conducted on each microstructure to optimize the finite element model size. Via a second Python script, the meshed microstructures were recreated in Z-set [14] in order to apply periodic boundary conditions and to compute their stiffness matrix .

2.2. Stiffness performance indicator

The works of Kanit [6] and of Hollister and Kikuchi [15], showed that the convergence behavior of a periodic microstructure is reached quickly, as its volume increases. The behavior of the biggest volumes was then considered as converged and a global behavior indicator, EC_G, of the microstructures was consequently defined thanks to the behavior of the biggest ones. The global indicator estimated the evaluation of the elastic performances from 0 to 1. Finally, the eighth microstructure of the $3L_f$-5% $5d_f$ class was retained due to its elastic performances equal to the convergence behavior.
For the following work on the local indicator, the entire class has been retained due to the presence of the SRVE and to its distribution of stiffness on the different microstructures, as shown in Table 1. Among the ten volumes of this class, seven had a stiffness behavior close to the convergence one (EC_G > 0,8), five were quasi-equal to it (EC_G > 0,9) and one was far off this target (the fourth one).

Table 1. Global performance indicators (EC_G) in the $3L_f$-5% $5d_f$ class of microstructures

Volume	EC_G
1	0,871
2	0,938
3	0,832
4	0,442
5	0,739
6	0,691
7	0,952
8	1,000
9	0,901

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10	0,927

3. Local indicator

In Table 1, only one of the ten generated volumes is perfectly reaching the convergence behavior. For that kind of microstructures, the computation of the stiffness matrix takes over 80 minutes with the full field computing chain presented in the previous part of this paper. Knowing that only the fiber positions are different in each volume, the morphology of the microstructure seems to be responsible for the macroscopic behavior. The local indicator presented in this part was built to understand the effect of the fiber positions on the global behavior of the microstructure. This indicator is based on the fiber vicinity in the microstructure. In the following part, the subscripts *S* and *V* are respectively linked to a slice and a volume.

3.1. Definition

The proposed approach is inspired by the works of Christensen [9] and Jean [10] on 2D periodic volumes. The fiber proximity in a considered microstructure induces a more or less important local matrix confinement. Given that the matrix confinement is directly linked to the mechanical behavior of the microstructure [16], the fiber position thus influences the macroscopic behavior. In order to extend these observations to 3D, each microstructure is discretized into 2D slices, cut in the length of the microstructure (
Figure **3**).

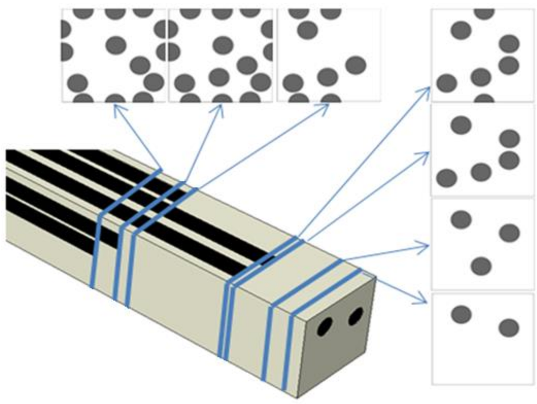

Figure 3. Slicing procedure of the 3D volumes

The thickness of each slice is conditioned by the beginning and/or by end of a fiber. Knowing the number of fibers N_f in the microstructure, the number of slices N_S is defined by: $N_S=2\,N_f+1$. Slices of known thickness, where the proportion and the position of the fibers don't change, are thus obtained and can be approximated as 2D surfaces. For each slice isolated with this method, a local indicator, based on the first neighbor distance of the fibers D_S, can be determined by the equation (1) :

$$\alpha_S = \frac{D_S \times T_S}{\left({Vol_S}/{Vol_V} \right)} \tag{1}$$

Where D_s is determined with a numerical MATLAB® [17] tool presented by Ghossein and Lévesque [18]. The first neighbor distance is thus defined as the closest distance between two fibers, considering their external envelope. Because of the periodicity of the microstructures, the first neighbor distance

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has to be computed has if the same microstructure is repeted on each side of it, as illustrated in Figure 4 for the both the left and bottom sides.

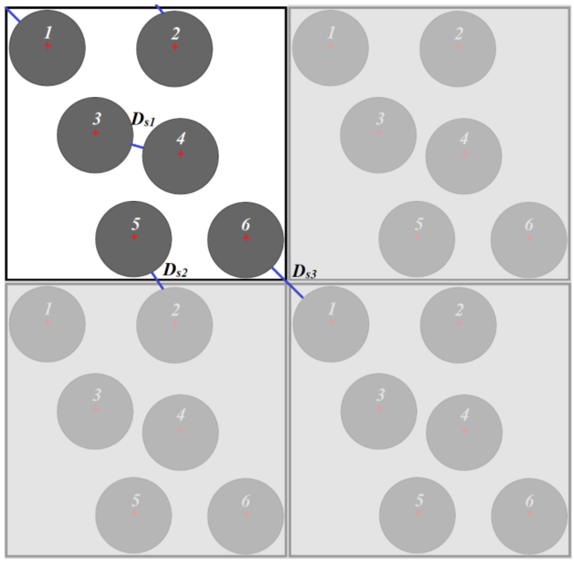

Figure 4. Determination of the first neighbor distance of the fibers in a periodic microstructure

T_S is the thickness of the considered slice, and Vol_S and Vol_V are respectively the volume of the slice and the entire volume of the considered microstructure. The ratio between the two volumes gives the proportion of the slice in the whole volume. The relation (1) thus gives the proportion of the maximum matrix confinement in the slice compared to the whole considered volume. The sum of the α_S in the entire volume gives α_V, which represents the matrix confinement level of the considered volume (in μm^2).

3.2. Application

In the following part, the local indicator of the microstructure is compared to the stiffness indicator indicated in part 2.2 for the retained class of microstructures. For this purpose, fifty new random microstructures of the retained class are generated, the stiffness matrix is computed and it allows the comparison between the global behavior of the microstructures (indicated by EC_G) and their matrix confinement level α_V (Figure 5).

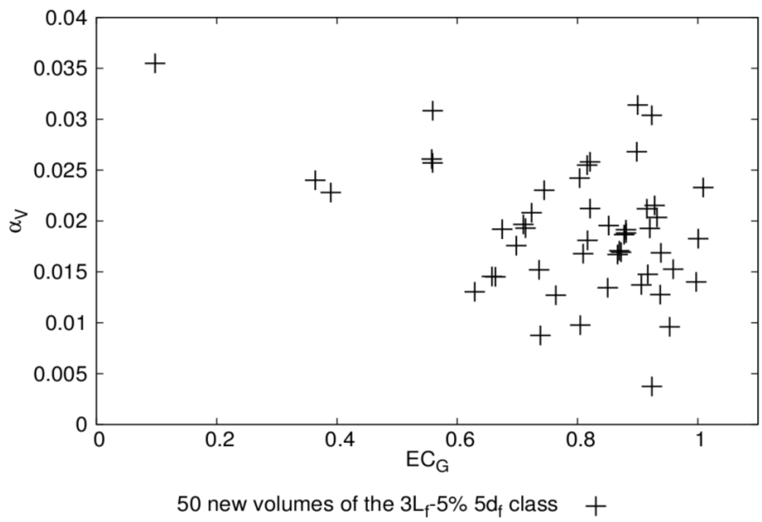

Figure 5. Relation between α_V and EC_G for fifty new 3D volumes

The plotted point cloud on the new volumes seems to show that the smaller α_V is, the more the considered microstructure has a chance to have a high EC_G. In other words, the less the matrix is confined, the more the global behavior of the volume can be close to the convergence stiffness. The matrix confinement can also be highlighted by the distribution of local volume fraction in a microstructure. To illustrate this principle, the distributions of volume fraction of the microstructures with the lowest and the highest α_V are computed in three equal sub-volumes (Figure 6).

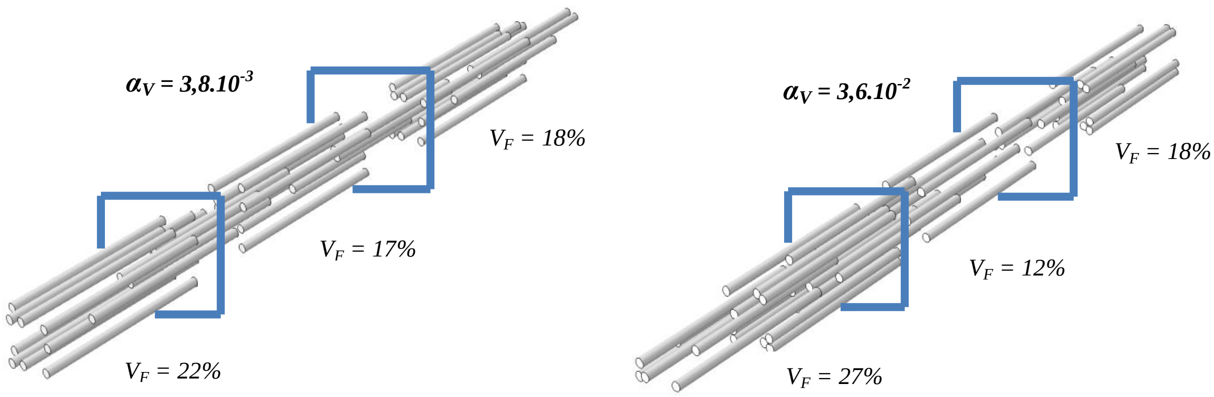

Figure 6. Comparison of the volume fraction distribution between two microstructures for a low (left) and a high (right) α_V

Regarding Figure 6, hight values of α_V traduces clustering or lack of fibers in the microstructure. The proposed verification of the relation between α_V and EC_G consisted in the generation of fifty new random microstructures, whose α_V is then calculated. The stiffness matrix and EC_G are computed for the microstructures with the ten lowest values of α_V. The aim of this verification is to confirm the possibility to estimate the global behavior of a microstructure thanks to its morphology. These results are presented in Figure 7.

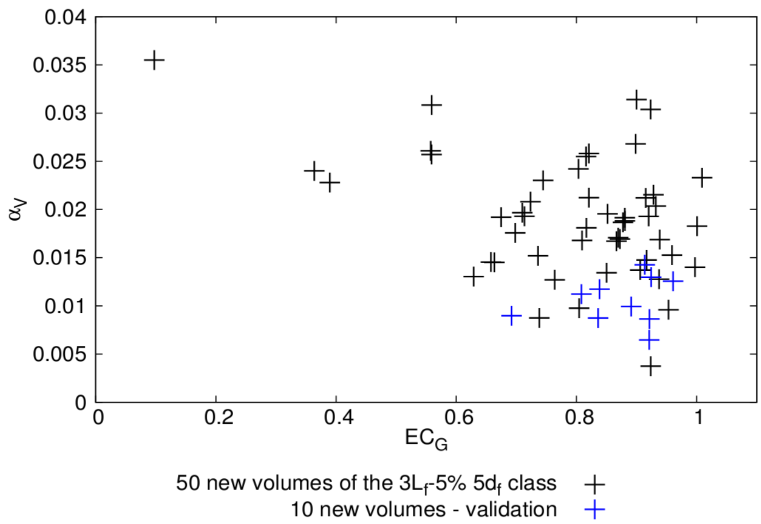

Figure 7. Convergence behavior of the ten validation microstructures

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The preselection of the microstructures through their matrix confinement level before the finite element computing gave a pertinent shortlist of microstructures. This preselection avoided several finite element computations for the acquisition of more accurate microstructures in terms of convergence behavior. The values of the EC_G and α_V are presented in Table 2.

Table 2. EC_G and α_V of the validation microstructures, classified in descending order of α_V

Volume	EC_G	α_V [µm²]
1	0,921	$6{,}472.10^{-3}$
2	0,922	$8{,}638.10^{-3}$
3	0,836	$8{,}742.10^{-3}$
4	0,692	$8.974.10^{-3}$
5	0,891	$9{,}939.10^{-3}$
6	0,808	$1{,}122.10^{-2}$
7	0,838	$1{,}174.10^{-2}$
8	0,961	$1{,}257.10^{-2}$
9	0,924	$1{,}297.10^{-2}$
10	0,914	$1{,}426.10^{-2}$

In the ten new generated volumes, nine have a stiffness behavior close to the convergence one (EC_G > 0,8) and five are quasi-equal to it (EC_G > 0,9). Although this method seems to be relevant most of the time, the fourth volume shows that it requires further examination in order to systematically generate an accurate SRVE.

4. Conclusions and perspectives

The determination of a SRVE is an important step for a more realistic behavior modeling of a short fiber reinforced composite. The proposed method deals with the definition of a local indicator of the 3D microstructure and constitutes a first step towards an understanding approach of the influence of a periodic RVE morphology on its stiffness behavior. The stochastic approach with the definition of the local indicator showed that the microstructural indicator could also be a help to shortlist potential RVEs, which could lead to a faster and more accurate definition of a RVE than a full classic method.

In future works, the integration of an additional statistic tool could help to confirm the pertinence of the microstructural indicator. The Integral Range, introduced by Matheron [19] and Lantuéjoul [20] in geostatistics, is a robust statistical tool based on the variance of a physical model. Like in the work of Escoda [21], it has been used for the determination of a RVE in a strictly statistical approach. For the presented work, it could allow to determine the number of necessary volume realizations to reach a fixed relative gap from the target behavior. In a second time, the extension of the microstructural indicator to non-linear computation would allow to confirm, or not, this approach.

References

[1] F. Gehring, Mechanical behavior and damage study of short hemp fiber reinforced thermoplastics : experimental approach and modelling, *PhD Thesis, Université de Lorraine*, 2013.

[2] R. Hill, Elastic properties of reinforced solids: Some theoretical principles, *Journal of the Mechanics and Physics of Solids*. 5: 357–372, 1963.

Excerpt from ISBN 978-3-00-053387-7

[3] A.A. Gusev, Representative volume element size for elastic composites: a numerical study, *Journal of the Mechanics and Physics of Solids*. 45: 1449–1459, 1997.

[4] M. Ostoja-Starzewski, Material spatial randomness: From statistical to representative volume element, *Probabilistic Engineering Mechanics*. 21: 112–132, 2006.

[5] H. Moussaddy, A new definition of the representative volument element in numerical homogenization problems and its application to the performance evaluation of analytical homogenization models, *PhD Thesis, École Polytechnique de Montréal*, 2013.

[6] T. Kanit, S. Forest, I. Galliet, V. Mounoury, D. Jeulin, Determination of the size of the representative volume element for random composites: statistical and numerical approach, *International Journal of Solids and Structures*. 40: 3647–3679, 2003.

[7] A. Megally, Study and modeling of fiber orientation in reinforced thermoplastics, *PhD Thesis, École Nationale Supérieure des Mines de Paris*, 2005.

[8] F. Rasselet, S. Joannes, J. Renard, E. Roche, S. Pautard, Modeling and definition of a statistically representative cell: application to a unidirectionnal short-fiber reinforced composite material, *Journal of Composite and Advanced Materials*, to be published.

[9] R. Christensen, *Mechanics of composite materials*, Wiley & Sons, 1979.

[10] A. Jean, Rubber with carbon black fillers : from nanoscopic structure to the macroscopic behavior, *PhD Thesis*, *École Nationale Supérieure des Mines de Paris*, 2009.

[11] S. Forest, *Milieux continus généralisés et matériaux hétérogènes*, Presses des MINES, 2006.

[12] E-Xstream, *Digimat 5.1.2 User Manual*, 2014.

[13] Simulia - Dassault Systems, *Abaqus 6.14.1 User Manual*, 2014.

[14] *Z-set 8.6 User Manual*, 2015.

[15] S.J. Hollister, N. Kikuchi, A comparison of homogenization and standard mechanics analyses for periodic porous composites, *Computational Mechanics*. 10: 73–95, 1992.

[16] P. Rochette, P. Labossière, Axial testing of rectangular column models confined with composites, *Journal of Composites for Construction*. 4: 129–136, 2000.

[17] MathWorks, *Matlab R2013a User's guide*, 2013.

[18] E. Ghossein, M. Lévesque, A fully automated numerical tool for a comprehensive validation of homogenization models and its application to spherical particles reinforced composites, *International Journal of Solids and Structures*. 49: 1387–1398, 2012.

[19] G. Matheron, *The theory of regionalized variables and its applications*, École nationale supérieure des Mines de Paris, 1971.

[20] C. Lantuéjoul, Ergodicity and integral range, *Journal of Microscopy*. 161 (1990) 387–508.

[21] J. Escoda, 3D Morphological and micromechanical modeling of cementitious materials, *PhD Thesis, Ecole Nationale Supérieure des Mines de Paris*, 2012.

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