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Statistical analysis of real and simulated fibre arrangements in unidirectional composites

Valentin Romanov *, Stepan V. Lomov, Yentl Swolfs, Svetlana Orlova, Larissa Gorbatikh, Ignaas Verpoest

Department of Metallurgy and Materials Engineering, KU Leuven, Kasteelpark Arenberg 44, B-3001 Leuven, Belgium

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ABSTRACT

Modelling of the onset and propagation of matrix cracks in fibre-reinforced composites on the micro scale requires adequate representation of the material microstructure. In the present work we compare simulated and real fibre arrangements found in unidirectional composites, using statistical descriptors. The comparison is done for geometrical and mechanical parameters such as distributions of the fibre positions and the stress fields. The real fibre arrangements are extracted from microscopy images of a 3D non-crimp woven carbon/epoxy composite with fibre volume fractions of 58–68%. The modelled fibre arrangements are generated using a heuristic random microstructure generation algorithm. The stress fields are compared for the case of transverse tension. A good correlation between statistical parameters of the real and simulated fibre arrangements is obtained.

1. Introduction

The damage development in high performance fibre-reinforced polymers is a complex process that unravels on different length scales and is intimately linked to the material internal structure. Microscopic damage in the form of fibre/matrix debonds and matrix cracks is an important stage towards composite failure, as it may trigger other failure modes such as delaminations and fibre breakage. The onset of the microscopic damage is known to depend on the local stress state, local fibre volume fraction and material properties of fibre and matrix. It is also sensitive to the spatial distribution of fibres.

Fibre arrangements in unidirectional (UD) composites are typically non-uniform and non-periodic. Effects of the non-uniform fibre distribution on the composite overall behaviour have been extensively studied in the literature [1–7]. It is generally agreed that periodic fibre distributions lead to incorrect predictions of the elastic–plastic behaviour under transverse loading conditions [8–10]. The microscopic stress distribution is highly sensitive to the fibre distribution while the macroscopic elastic effective response of a laminate may not be affected by it [11]. Damage evolution is strongly affected by inter-fibre spacing [12]. Fibre arrays are found to be significant contributors to matrix cracking causing local stress concentrations and strain localization [13]. It is, thus, concluded that an adequate prediction of the stress distribution and analysis of damage on the micro-scale requires a "true-to-life" representation of fibre arrangements.

The most straightforward way to create a representative volume element (RVE) of the fibre distribution is to use experimental data, for example, from microscopy images of composite cross sections [14–17]. This approach, however, can be time and resource consuming; it requires specific software and hardware for image acquisition and processing. The number of available realisations by the available experimental dataset is also usually limited.

The other approach is to simulate fibre distributions based on a certain numerical algorithm. In the literature, the problem of the fibre distribution generation is reduced to the problem of spatial in-plane point processing under several conditions. The first condition is that fibres cannot intersect each other, translating into a minimum distance between the centres of the fibres. The second condition is that a given volume fraction must be reached. The Poisson point distribution [18], which provides a uniform statistical distribution of points with exactly the same probability of finding a point near any coordinate of the area of interest, is not appropriate for this, since it does not guarantee non-overlapping fibres. There are many models that overcome this difficulty [19]. One of them is the Strauss "hard-core" algorithm [9,18] that creates a random distribution of points with the condition that no pair of points may be closer than a certain minimal distance. This algorithm, however, does not work for fibre volume fractions higher than 50…55% [20,21]. In some algorithms [1,22–24], a high fibre volume fraction can be achieved by generating fibre placements via perturbation of an initially regular periodic packing. Jodrey and Tory [25] proposed an algorithm to generate a random

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* Corresponding author. Tel.: +32 16321319.
E-mail address: Valentin.Romanov@mtm.kuleuven.be (V. Romanov).

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distribution of spheres in 3D, which can be used in 2D problems for the distribution of circles.

The proposed methods for generation of fibre distributions are readily applicable as a pre-processor for finite element modelling, for example, to predict stress distributions and crack propagation. It, however, remains unclear whether the simulated microstructures are equivalent to real microstructures. The equivalence is understood here in the sense that it correctly represents not only the overall fibre volume fraction but also statistical characteristics related to spatial positions of fibres and stresses generated when this material is mechanically loaded. The spatial position of fibres in a composite is influenced by the conditions of the composite production: applied pressure, matrix flow, geometrical constraints of the mould, etc. These conditions may lead to fibre clustering and formation of resin rich zones, features that need to be properly modelled in the RVE to be used for further modelling of damage. Most of the available algorithms are not statistically analysed for this purpose. Vaughan and McCarthy [26] proposed a method of generating fibre arrangements based on correlation functions that characterize experimental distributions. This method has not been validated yet in mechanical modelling and may be biased because of the choice of an experimental set.

From this literature review we conclude that there is a need for a fibre placement generation method, which would (1) generate fibre distributions with "true-to-life" statistical characteristics, and (2) be capable of producing distributions with high (60...70%) fibre volume fractions. The recent method proposed in Yang et al. [27] is able to generate fibre distributions with high fibre volume fractions. It was also statistically analysed on its equivalence to real microstructures, but the predicted elastic properties as well as some geometrical correlation functions did not correlate well with experimental data.

The random microstructure generation (RMG) algorithm proposed in Melro et al. [28] is also capable to simulate microstructures with high fibre volume fractions. Additionally, it was shown to provide a better computational performance and to generate fibre arrangements that are statistically closer to the Poisson random point distribution than the ones generated in [1,11]. However, even when the general criteria of randomness are satisfied, it is not yet certain whether the fibre placement algorithm ensures that the generated fibre distribution has statistical parameters close to those of real fibre distributions. The inhomogeneity of the fibre distribution in real composites such as local fibre clustering introduces extra stress gradients, which are expected to play an important role in the onset of damage. Therefore, mechanical factors such as stress concentrations should be investigated and the equivalence between stress fields in real and simulated microstructures should be demonstrated.

In this work, we investigate whether the RMG algorithm creates fibre arrangements that are statistically equivalent to those found in UD composites.

2. Problem statement and methods

The aim of the present work is to assess the statistical equivalence between fibre distributions reconstructed from microscopy images of real composites and those generated using the RMG algorithm. This analysis is performed on nine image-based reconstructed RVEs extracted from experimental data and nine simulated RVEs with the same fibre volume fractions. The two sets of fibre distributions are then analysed for statistical equivalence. The statistical equivalence is defined here twofold as (1) equivalence of distributions of the fibre positions (in geometrical definition), and (2) equivalence of statistical parameters of stress fields (in mechanical definition).

2.1. RMG algorithm

The algorithm is only briefly introduced here. The reader is referred to [28] for its detailed description. The algorithm is divided in three sequential steps:

1. The first step is a hard-core algorithm, where fibre centres are randomly generated inside an RVE. Input variables are the fibre radius, the dimensions of the RVE and a minimum distance between fibres. The hard-core model guarantees that there is no overlapping of fibres, but it is impossible to reach fibre volume fractions higher than $\sim 55\%$.
2. The second step is a heuristic rearrangement of the fibres. It is an iterative step and is invoked if the specified fibre volume fraction has not been reached in step 1. Depending on the iteration number, each fibre defines the closest, second closest or third closest fibre and then shifts position of its centre towards a chosen fibre by a random distance between 0 and the maximum distance allowed to avoid fibre intersection. This process is applied to every fibre once per iteration and creates open spaces between the fibres all over the RVE. The freed spaces will be used to place new fibres in step 1 of the next iteration.
3. In the last step the fibres positioned along the edges of the RVE are pushed inwards, always saving the minimum distance between fibres and not overlapping. The sequence of these three steps is then repeated until the required fibre volume fraction is reached.

A MatLab code, provided by the authors of [28], was used in the present work with the following modification. In the original algorithm the minimum distance between the fibre centres is constrained to $2R$, where R is the fibre radius. We have found that this leads to an unrealistically high number of fibres touching one another in comparison with the experimental fibre distributions. In UD composites, a tiny gap almost always exists between the fibres due to very low but still tangible fibre crimp in longitudinal direction. In our calculations the minimum distance between the fibre centres is a randomly chosen variable for each fibre pair that lies in the interval $[2R, 2.1R]$. This modified version of the RMG algorithm is further called simply "the RMG algorithm". The algorithm is efficient, it requires only several seconds to achieve a fibre volume fraction of 60%. A fibre volume fraction of 65% is achieved in less than a minute. All runs were performed on a laptop computer with an Intel(R) Core(R) i7 1.87 GHz processor, 8 GB of RAM memory and hyper-threading turned ON.

2.2. Image-based reconstruction of fibre distributions

Real fibre distributions are reconstructed from microscopy images of yarns in a 3D non-crimp woven carbon/epoxy composite [29]. Yarns taken from the middle of this composite can be considered unidirectional due to a very low crimp (less than 0.3%). The fibre diameter was measured to be $d_f = 6.93 \pm 0.27$ μm. Nine optical high magnification micrographs (0.073 μm/pixel) from inner regions of warp and fill yarns shown in Fig. 1 were used for analysis in this work. Three of the micrographs were taken from "warp-2" ($V_{f1} = 62.5\%$, $V_{f2} = 66.4\%$, and $V_{f3} = 64.6\%$), three from "fill-2" ($V_{f4} = 64.3\%$, $V_{f5} = 60.1\%$, and $V_{f6} = 61.3\%$) and three from "fill-3" ($V_{f7} = 62.2\%$, $V_{f8} = 57.6\%$, and $V_{f9} = 67.9\%$). V_{fi} indicates the corresponding fibre volume fractions. Based on these images nine 2D RVEs of a size 223.5 × 223.5 μm were constructed. The RVE consists of $\sim$200 fibres and is considered as representative both geometrically and mechanically according to [30,31]. The diameter of all fibres is assumed to be equal to the measured average (6.93 μm). For brevity this experimental set of fibre distributions is called an "experimental set (ES)". The coordinates of the fibre