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Toward better understanding of the effect of fiber distribution on effective elastic properties of unidirectional composite yarns

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ABSTRACT

A combined X-ray micro-computed tomography (XMT) and micro-Finite Element Analysis study is presented to quantify the effects of micro-scale random fiber distributions on the effective (homogenized) elastic properties of unidirectional (UD) yarns, as often used by designers for component-level computational modeling of composite structures. In addition, it is shown how the XMT artefacts can yield unreliable FE homogenization of the composite yarns by overestimating the stress transfer capacity between the material constituents. Finally, the micro-FEA modeling results under fiber distribution randomness are compared to the macro-level predictions such as the classical rule of mixture and Halpin–Tsai equations.

1. Introduction

Long-fiber reinforced polymers have gained significant attention in many industrial applications because of their low density, high specific stiffness and strength, and low thermal expansion [1]. Such composites are inherently multi-scale materials since their properties at the macro-scale are strongly affected by their fiber architecture and behavior at lower scales. In general, a composite material has three distinguishable scales: (i) macro-scale which normally refers to a manufactured part, (ii) meso-scale which is an intermediate scale and refers to the yarn architecture, and (iii) micro-scale which concerns the assembly of a large number of fibers that make up an individual yarn [2].

Over the years, numerical simulation tools have been extensively utilized to investigate the behavior of composites at different material scales [3]. One area of interest has been the prediction of macro-mechanical properties using micro-mechanics modeling, based on the known properties of the matrix and the reinforcement material phases [4]. This method is normally preformed through the analysis of a representative volume element (RVE) or a unit cell [5–7]. For different types of composites (e.g. unidirectional and textile composites), the mechanical properties of the material macrostructure can be simulated by periodically repeating such unit cells. Focusing on the case of unidirectional lamina, the repeating unit cell has been often defined in the literature assuming that the reinforcement has a uniform distribution and identical geometry [4]. However, not all the reinforcing phase constituents necessarily have the same geometry. In the case of glass fiber reinforced polymers (GFRPs), for example, depending on the supplier of the raw material, the fibers can have very different radii and the arrangement of fibers within the matrix is often non-periodic. Although these micro-level uncertainty effects will vary the properties of composite part at the macro-level [2], the available simulation tools do not often take such material inhomogeneity into account [8,9], and designers in industry use average macro-material properties from given datasheets/handbooks. However, to obtain an accurate and reliable virtual model of a composite part at macro-level, the statistics of the microstructure must be characterized and incorporated using microscopy of actual specimens and a multi-scale analysis framework [10].

Due to advances in computer sciences and image processing technologies, image-based modeling, in which detailed models of specimens are created based on realistic geometry acquired via microscopy, has made significant advancements in the last decade. Three-dimensional (3D) image-based modeling is today possible using X-ray micro-computed tomographic microscopy (XMT) machines for image acquisition, followed by image processing and meshing using available software such as ScanIP™ (Simpleware, UK). The combination of XMT and image processing tools is a useful technique for modeling of complex hierarchical materials such as composites [11]. Blacklock et al. [10] have used statistical data obtained from XMT to generate virtual textile

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composite specimens rather than using the XMT image directly. More specifically, the textile reinforcement was presented as one-dimensional tow loci in 3D space, which was then incorporated into a binary model of textile composites. Simulation and XMT analysis of textile composite reinforcement deformation (e.g., biaxial tension and in-plane shear) at the mesoscopic scale was performed by Badel et al. [12] to characterize the 3D geometries of the deformed and un-deformed reinforcement, and particularly to provide a correct fiber distribution within a yarn model. In another study, Alghamdi et al. [11] presented a multi-scale 3D image-based model of a carbon/carbon (C/C) composite to evaluate its thermal diffusivity and Young's modulus. Specifically, two finite element (FE) models were created at different length scales; the micro-scale model was developed from scanning electron microscope (SEM) micrographs of the carbon tow, while the macro-scale model was developed from XMT images of the composite. The use of XMT images to create an image-based model of composites is advantageous because, due to its non-destructive nature, the XMT technique prevents the internal microstructure/features from being affected by sample preparation stages such as cutting of the specimen. However, a disadvantage in an image-based model of polymer-matrix composites is the similar absorption coefficients of the fibers and matrix phases, leading to similar grayscale levels and thus making fiber segmentation difficult [11]. The micron level spatial resolution of XMT images may also make it challenging to properly separating adjacent fibers, depending on the fiber diameter.

As outlined above, finite element (FE) modeling at the micro-level can be used to estimate the mechanical properties of a composite part at a macro-level; which is normally the level used by most designers in industry. On the other hand, the heterogeneity is an essential/inherent characteristic of composite materials [13–23]. Thus, 'homogenization' through numerical methods (e.g., FE) has been implemented by researchers as a capable method for predicting properties of the material in higher scales using results of analysis in lower scales. Homogenization starts by considering an RVE that is a subsystem of the entire composite part and can represent its typical structure fairly well [13–15]. For composite parts with an ideal periodic media, defining this unit cell is rather easy. However, the reality of fibers' random distribution inside the matrix is more challenging. In general, the selected RVE should include a reasonable number of micro-level features and represent overall fiber distribution. The effect of micro-level random features during homogenization of composites along with the effect of RVE size has been scarcely studied in the past.

In the present study, a combined XMT-FEA investigation has been carried out to characterize the effects of micro-scale fiber spatial distribution on the overall mechanical properties of a typical unidirectional (UD) fiberglass/polymer composite yarn. First, XMT has been used to image a consolidated UD yarn containing glass fibers. Then, a series of finite-element simulations were carried out on both randomized micro-scale RVEs (hereafter called "Randomized Unit Cell Analysis Library" or R-UCAL), as well as a full-size scanned macro-scale yarn specimen. Although many other uncertainly variables could be considered, *the focus of this work is to characterize the effect of fiber radii as well as fiber centroid distribution on the ensuing effective properties of consolidated UD yarns at different volume fractions, when compared to theoretical (average) predictions*. The assessment of the FE models generated by random reinforcement phases immersed in the matrix, versus those meshed based on the computed micro-tomography scans of the real material microstructure, has also been the topic of recent studies, although on different types of materials and properties (e.g., on a Cr–Al_2O_3–Re composite and its Young's modulus [24], or on a random chopped fiberglass composite and its Young's modulus as well as in-plane shear modulus [25], or on a short steel fibers composite and its equivalent orientation tensor [26]). Also recently a new approach for compressing and reconstructing complex information on the two-dimensional microstructures of disordered (random) particulate media has been introduced [27], by means of a finite set of tiles assembled via a stochastic tiling algorithm. The current case study has selected a long-fiber reinforced thermoplastic (LFRT) material along with the five elastic properties that are needed for its macro-level three-dimensional FE analysis as a transversely isotropic UD composite.

2. Methodology

2.1. X-ray tomographic microscopy

X-ray micro-computed tomography (XMT) was performed on a unidirectional (UD) yarn containing glass fibers embedded in polypropylene matrix, using a MicroXCT-400 (Zeiss™) instrument in order to visualize fiber distribution. During the XMT set-up, 2500 2-D radiographic projections were acquired at different angles through 360° at an exposure time of 25 s for each radiograph. The projections were reconstructed to create a tomographic volume containing $1600 \times 1600 \times 500$ voxels at a voxel size of 0.53 μm. The volume image was then post-processed to separate the fiber and matrix phases and to extract geometrical information about the fiber distribution within the yarn using the advanced ImageJ and Avizo® packages. Due to imaging a UD yarn, all the cross-sectional slices were comparable. Thus, only a single slice, shown in Fig. 1, was used for further analysis.

2.2. Finite element analysis of R-UCAL

2.2.1. Geometry and mesh

A series of small representative volume elements (RVEs) with a fiber volume fraction ranging from 0.14 to 0.54, shown in Fig. 2, were randomly extracted from the XMT image of Fig. 1 for the consolidated PP/glass UD composite yarn, in order to establish a Randomized Unit Cell Analysis Library (R-UCAL) with cell size of 150×150 pixels (0.08×0.08 mm). For each library element (i.e., individual unit cell as an idealized binary image similar to the study [28]), the coordinate and radius of individual fibers were extracted using a digitizer software (xyExtract) and an in-house developed Matlab® code, and then regenerated in Abaqus® as an FE mesh. 3D continuum elements were used to discretize the library elements.

2.2.2. Simulation procedure

In order to simulate deformation of the library elements, a series of finite element models was created and analyzed using the commercial FE package SIMULIA Abaqus as follows. The mechanical simulations were performed under the assumption of small deformation theory. It must be noted that the theoretical grounds laid down in subsequent subsections are suitable particularly when using commercial software. When building own in-house FE software, the formulation may be provided in a simpler way, e.g., without giving special attention to the Poisson's ratio and shear stiffness effects [29], depending on the geometry or loading condition of structure.

(i) ***Periodic boundary conditions***

The boundary conditions that are applied to imitate the adjacent repetitive cells in RVE modeling are called periodic boundary conditions (PBCs) [15]. The basic principle of a periodic boundary condition relies on the fact that from a micro-level point of view, each point on one side of the RVE undergoes deformation identical to the point on the opposite side. In this way, an RVE can be used to