MICROSTRUCTURE-BASED MODELING OF THE CREEP BEHAVIOR OF LONG-FIBER-REINFORCED THERMOPLASTICS

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Abstract

Aim of this work is the prediction of the creep behavior of long-glass-fiber-reinforced polypropylene by microstructural simulations. This paper describes the generation of representative volume elements (RVE) for finite element simulations (FEM) employing a novel approach which takes into account the consolidation process of the composite during fabrication. First, a stack of straight fibers is generated according to the experimentally measured orientation distribution, then the compression of the fiber stack is numerically simulated and finally the remaining pores are filled with matrix elements to form the RVE. The resulting orientation distribution of the RVE is compared with measurements from computer tomography and shows excellent agreement. The capabilities of the FEM model are demonstrated by comparison of the elastic properties of the composite to experimental measurements.

1 Introduction

Today's efforts to achieve environmental compatibility while maintaining individual mobility result in a demand of medium to high performing and still economically producible materials for automotive applications. Long fiber reinforced thermoplastics (LFT) can meet a wide range of those criteria. The innovation cluster KITe hyLITE of the Fraunhofer society and the Karlsruhe Institute of Technology deals with the development of production processes and assessment methods of modern, mass producible composites such as LFT. While the quasi-static mechanical properties of LFT are known to some extent, larger uncertainty persists regarding the creep behavior. Hence, the aim of the current work is the prediction of the creep behavior as a function of the microstructure, characterized through its fiber volume content, fiber orientation state and fiber length distribution. This paper deals with the generation of a representative volume element (RVE) for PPGF30 (30 mass-% glass fiber reinforced polypropylene) with fiber lengths up to 50 mm.

2 Materials and methods

2.1 LFT-D process

The German company Dieffenbacher and the Fraunhofer ICT developed a LFT direct process where the fiber rovings break in the extruder instead of being introduced in a pre-cut form by means of the polymeric granulate [1]. The material is therefore called LFT-D. The resulting maximum fiber length of well above 20 mm up to 50 mm yield excellent structural properties which, in combination with a highest-degree freedom of design, makes the process as well as the materials attractive for structural applications. Different combinations of fibers and matrix are possible. Only polypropylene (DOW® C711-70RNA) with 30 mass-% glass fibers (TufRov® 4575) is regarded in this work.

The material's properties strongly depend on the microstructure. This microstructure locally varies in the LFT-parts. For the current work, 3 mm thick plates with outer dimensions of 400 x 400 mm have been produced by compression molding. The LFT-D strand as it comes out of the extruder was placed asymmetrically in the mold to separate the so-called press region near the strand inlay position from the flow-region, where a lateral streaming is responsible for a higher degree of fiber orientation compared to the press-region.

2.2 Mechanical testing

The unidirectional stiffness under tensile loading of specimens with different fiber orientations, but similar fiber volume fractions and fiber length distributions was determined with a Hegewald & Peschke "Inspekt 100" testing machine. The specimen geometry was chosen according to DIN EN ISO 3167. The tests were performed at a strain rate of approximately 0.00022 1/s to a maximum stress of 10 MPa to make sure that no damage occurred. Three loading-unloading cycles per specimen were performed. The stiffness is taken as the mean value of the three loading cycles. At least three specimens per orientation were tested.

2.3 Microstructure analysis

Microstructure analysis has been performed on specimens from different regions of a 3 mm thick LFT-plate. The specimens for computer tomography (CT) have been prepared from similar regions as the specimens for mechanical testing were taken from. The tomography scans have been performed on a Phoenix "nanome|x 180NF" with a voxel size of 5 - 8 µm, depending on the specimen size. So the complete plate thickness could be analyzed with one scan. The data was analyzed by FiJi/ImageJ's plugin "Directionality" [2] after binarizing the raw voxel data and converting to a stack of 2D-images. Orientation histograms for each image of the stack have been extracted by the software in the plane perpendicular to the thickness direction, where most of the fibers are aligned. The resulting orientation distribution for the whole stack has been generated by summing up the single histograms.

2.4 RVE generation

As the fibers show a very large aspect ratio of up to 3000 (50 mm length, 17 µm diameter), all common approaches to model the fibers as straight cylinders and place them into a volume by random sequential adsorption (RSA) or Monte-Carlo-algorithms are problematic. The dependence of the achievable volume fraction on the aspect ratio for cylinder-shaped inclusions under the constraint of non-intersection has been discussed in [3] extensively, interpreting analytical, numerical and experimental results from various authors. Common agreement is that the maximum volume fraction for moderate aspect ratios of 80 will be in the region of only 10%, while here 18-25% are needed for an aspect ratio of up to 3000.

The approach taken here therefore mimics a consolidation process. The mesh of a single, straight fiber is copied multiple times and accumulated to a fiber stack according to the experimentally measured orientation distribution in the x/y-plane perpendicular to the thickness- or pressing-direction. The lateral offset in the x/y-plane is chosen randomly. This stack generation is performed using a custom-made FORTRAN-tool. In the next step, the fiber stack is compressed via an explicit FEM-simulation by ABAQUS® 6.11 under presence of general contact (considering additional spacing between the fibers) until the desired volume fraction is achieved. Matrix elements are not considered at this stage. The use of contact constraints permits the formation of a realistic structure. To retain the original fiber orientation state as best as possible, the compression is performed in two steps. First, all nodes of the fiber mesh are fixed in the x/y-plane and only have a degree of freedom in the pressing direction. Secondly the nodes are released and the consolidation procedure continues.

In the final step of the numerical consolidation procedure, the deformed fiber mesh is cut into a cuboid volume which represents the RVE boundary. The remaining volume is filled up with a tetraeder-mesh, optionally after inserting cohesive-zone-elements in between fiber and matrix. This last step is performed by Altair's HyperMesh, choosing the deformed fiber-mesh as "fixed elements".The RVE generation scheme is shown in Figure 1.

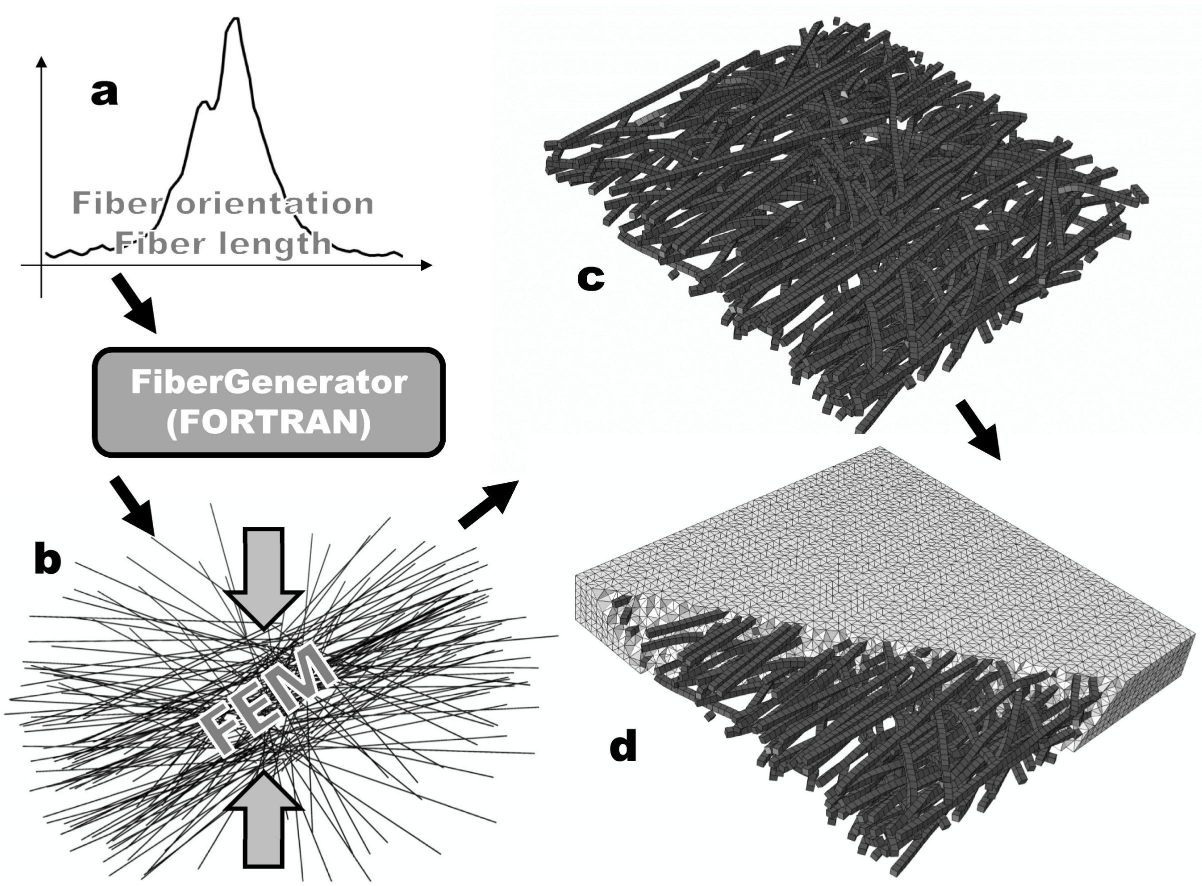

Figure 1. RVE generation scheme: Based on microstructural data (a) a stack of straight fibers (b) is generated and compressed by FEM until the desired volume fraction is achieved. The deformed fiber mesh is placed into a cuboid volume (c) before the remaining space is finally filled up with matrix elements (d). Dimensions of the shown RVE are 1x1x0.1 mm³. The number of elements is approximately 180 000.

3 Results

3.1 Mechanical testing

The mean stiffness values of at least three specimens per orientation are listed in Table 1. It is clearly shown that the stiffness strongly depends on both the specimen orientation and the region of the LFT-plate.

Plate section	**Specimen orientation**	**Stiffness [MPa]**
Press region	90°	3772
Press region	0°	6492
Flow region	90°	3251
Flow region	45°	3767
Flow region	30°	4313
Flow region	0°	7834

Table 1. Stiffness of tensile specimens from different regions and orientations (mean values of 3 loading-unloading-cycles).

3.2 Microstructure analysis

In Figure 2 (left), a schematic LFT plate with flow and press region as well as the corresponding CT-scans (middle and right) is shown. A different degree of orientation in x-direction (0°) can be observed visually in the 3D-views as well as the layered type of structure which justifies to only consider the orientation state in the x/y-plane for the RVE.

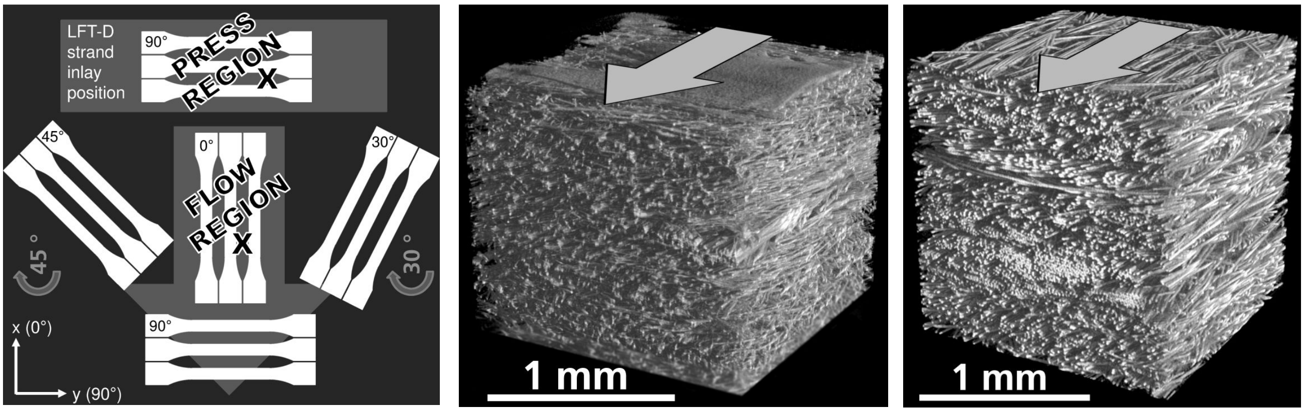

Figure 2. Schematic LFT plate with press and flow region (left). The positions for tensile specimens as well as for CT analysis (marked with an X) are highlighted. The resulting CT-scans for press (middle) and flow (right) region show different amounts of fibers aligned in 0° direction, marked with the grey arrow. The voxel size is 8 µm for the press region specimen and 5 µm for the flow region specimen.

In Figure 3 the corresponding orientation distributions generated by image analysis software can be found. The distributions are in good agreement with visual observations of the 3D images from Figure 2.

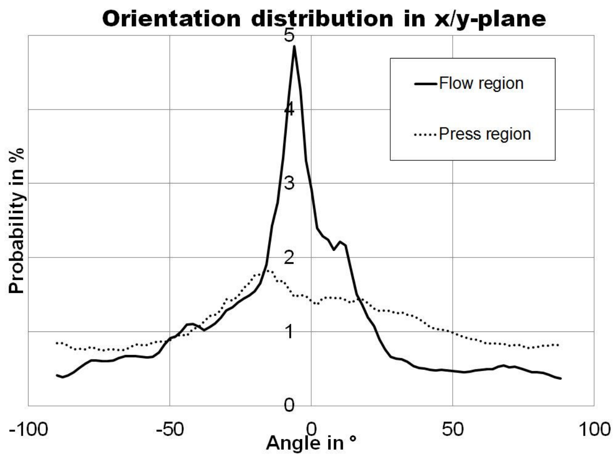

Figure 3. Orientation histograms for press and flow region in the x/y-plane as determined from image analysis of CT data.

3.3 RVE simulation

In the following, the FE mesh of three different RVEs was processed applying the same image analysis method as for the CT data. All RVEs had outer dimensions of 1x1x0.1 mm³, a fiber count of approximately 200 and contained about 180 000 elements. The fiber length distribution was considered to be homogenous. Fibers have been cut at the RVE boundary. All RVE models have been given the orientation distribution of the flow region (either in original or modified form). The RVE orientation distributions are depicted in Figure 4.

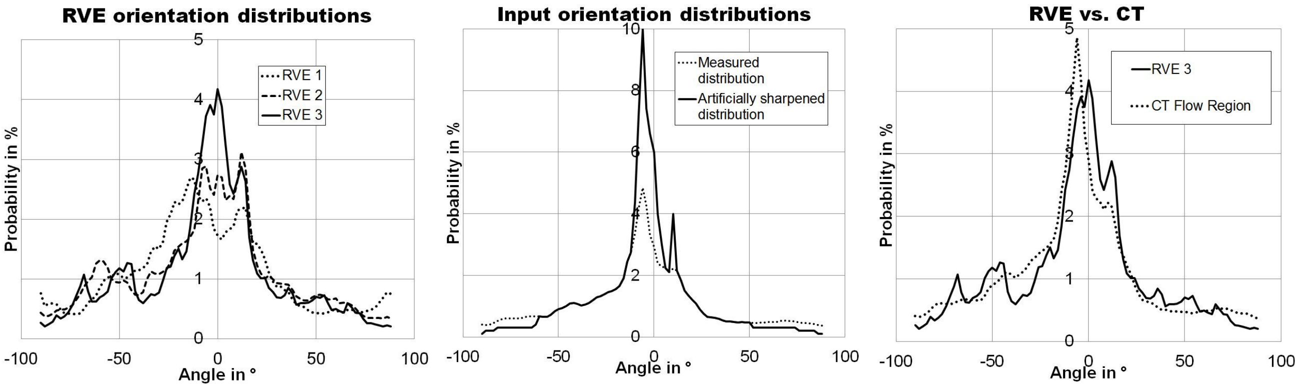

Figure 4. Orientation distributions for three flow region RVE variants (left), correspondent input distributions for the FiberGenerator tool (middle, please note the different scale of y-axis) and comparison of RVE 3 with the measured CT distribution (right).

In Table 2 the stiffness values of RVE simulations by ABAQUS® 6.11 Standard (implicit) are shown. Virtual tensile tests under extraction of the reaction forces of the displaced nodes have been performed.

Variant	E_{0° [MPa]	E_{90° [MPa]	E_{0°/E_{90°	v_f [%]	E_{Matrix} [MPa]
Experimental	7834	3251	2.41	ca. 17.7	-
RVE 3*	7717	3234	2.39	18.1	1400
RVE 3	7392	2962	2.50	18.1	1250
RVE 2	6820	3262	2.09	18.7	1250
RVE 1	6960	3728	1.87	18.9	1250

Table 2. Comparison of experimental and FEM results. The fiber properties were chosen as E_{Fiber} = 72 000 MPa and ν_{Fiber} = 0.22; the matrix Poisson ratio was ν_{Matrix} = 0.35.

The orientation distribution of RVE 1 as shown in Figure 4 left, generated with the original measured input distribution, shows a fair agreement to the measured flow region distribution from Figure 3. However the angular position of the peak slightly differs and the distribution is obviously flattened. This results from the issue mentioned in section 2.4 that the fiber fixation in the x/y-plane has to be released at a specific time during compression in order to enable further consolidation to higher volume fractions.

RVE 2 was therefore generated with the help of an artificially sharpened input distribution as it is depicted in the middle graph of Figure 4. The resultant orientation distribution (Figure 4, left) is still not sharp enough. This is probably due to inertial effects upon release of the fixation and too low glide resistance of the fibers.

As a consequence RVE 3 is not only generated with the artificially sharpened input distribution but also by adding a velocity in 0°/x-direction to the fiber nodes during the last phase of the compression procedure and by adding a static friction coefficient of 0.3 to the contact properties. Fiber warping is now significantly reduced and the agreement with the original fiber orientation distribution is very good, as shown in the right graph of Figure 4. Moreover, the introduction of a lateral velocity during compression is in agreement with the physical fabrication process at least for the flow region of the LFT plate.

The resultant stiffness values of virtual tensile tests performed with the RVE variants shown in Table 2 are in excellent agreement with values which can be expected based on the evaluation of the respective orientation distributions. The elastic properties of the fiber and matrix components are taken from literature. The matrix modulus coming from the manufacturer's data sheet [4] is referred to as a flexural modulus according to ISO 178 (no tensile value is given). However, comparing the stiffness of RVE 3 with experimental results, the matrix modulus value of 1250 MPa seems to be too low. Numerically a value of 1400 MPa for variant RVE 3* gives good agreement with the experimental data. A first tensile test on a pure matrix specimen gives a modulus of 1632 MPa. Since a matrix substance specimen will certainly not have the same properties as the matrix component of the composite, as the polymer microstructure differs, the numerically determined value seems reasonable.

An uncertainty remains for the "experimental" values of the fiber volume fraction. Considered here is a calculated value derived from process parameters during fabrication as the mass flow rate of the polymer and the roving length per unit time. Radtke [5] determined the mass fraction of plates from a similar material (LFT-D PPGF30 with pre-cut fibers) by weighing incinerated specimens from different plate regions. The maximum observed deviation from the nominal mass fraction was approximately 7 %. Transferred to the current studies, the volume fraction could vary between 16.6 and 18.9 %. Thus, the value of 18.1% of RVE 3 can be considered as realistic.

4 Discussion and outlook

A novel method to generate RVEs for LFT and similar materials has been developed and analyzed in detail regarding the resulting fiber orientation distribution and volume content. The method is appropriate to model a realistic structure of the considered material. Comparison with experimental measurements shows excellent agreement regarding the elastic properties.

Up to now, fiber length distribution has not been considered. For an assessment of the elastic properties, the length distribution can indeed be neglected if the majority of fibers is longer than about 0.2 - 0.3 mm [5,6,7]. This is the case for the randomly chosen length distribution in the current studies (the starting point for fiber extrusion in the x/y-plane is chosen randomly and the fibers are cut at the RVE boundary).

For strength predictions the critical fiber length roughly estimated according to [6,7] should be in the range of 1 - 2 mm for the LFT material. This supports the authors current assumption that it will be possible to predict the creep properties of the composite with a RVE size in the range of 2 - 8 mm edge length. This will cover the most important part of the fiber length distribution and a few longer fibers will probably not affect the creep properties significantly. With the presented RVE generation method it should be possible to create RVEs of the required size of several millimeters edge length taking into account the experimentally measured fiber length distribution from specimen incineration. The RVEs are well able to represent such large structures because of their very reasonable number of elements: Although the fibers are only modeled with one element over the cross section, a realistic microstructure with fiber crossings and entanglements resulting from the consolidation process is formed. Feasibility studies on RVEs of 1x1x0.1 mm^3 and approximately 180 000 elements with implemented viscoelastic matrix behavior lead to computing times of about 45 minutes with four processors relating to a time period of equivalent creep tests of one month. Most likely, far larger RVEs will also be processable in a reasonable time. However, it should be mentioned that the RVE generation process is far more costly.

Furthermore, feasibility studies to implement cohesive elements between fiber and matrix in order to be able to cover the interface properties have been performed. The mechanical behavior needs to be determined inversely or calibrated on micromechanical tests, as single-fiber-push-out.

A weak point of the described method is the coarse representation of the fiber's cylindrical cross-section by a single square element. Other methods that model a small RVE volume of typically 200 - 400 µm edge length often use a multitude of elements per fiber cross section (i.e. by directly mapping CT-data to a voxel-based mesh or by artificial generated structures based on a voxel- or surface-mesh). However, these approaches are not able to cover the fiber length distribution because of the excessively vast element count or the inappropriate use of periodic boundary conditions.

Similar to the different susceptibility of elastic and creep properties to fiber length, different aspects of the complex LFT microstructure need to be considered separately at different levels of discretization and for different application scenarios. This requires a multiple-step, multiple-scale homogenization procedure ranging from very small, but detailed RVEs with a voxel- or surface-mesh for exact predictions of the stress and strain fields in particular at the fiber ends to methods like the one presented here which are suitable to at least partially account for the influence of the fiber length distribution.

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