PREDICTING THE 3D ELASTIC-PLASTIC BEHAVIOR OF POLYMER-BASED FILTER MEDIA

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ABSTRACT

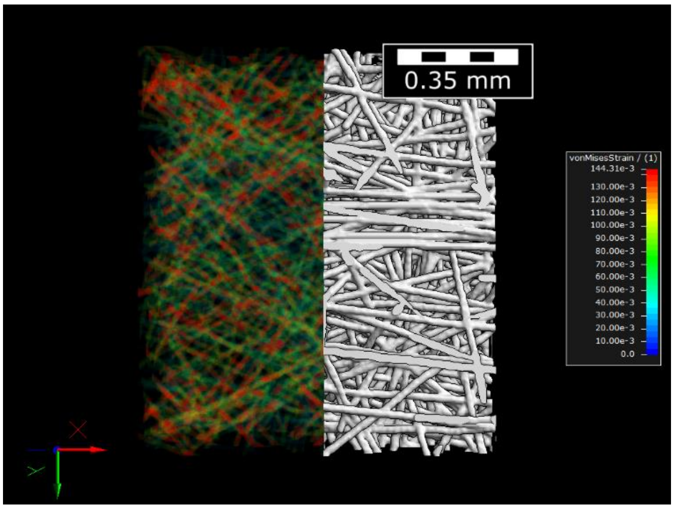

Fig. 1: Equivalent strain field of a polymer-based nonwoven filter media for the in-plane shear load case.

New filter media are developed to increase filtration performance based on simulations and parameter optimizations. In order to achieve the volumetric flow rate required by the application, it is often necessary to pleat the filter media. However, the highly anisotropic material behavior of these nonwovens is challenging. At this point in the design process of the new media, the microstructure's effective mechanical properties are unknown. The capability to predict these mechanical properties is crucial to assess the new microstructure's viability for further processing. Hence, a simulation model to test the virtual microstructural designs for tension, compression, and shear in all three spatial directions is needed.

This presentation introduces a microstructural simulation model to predict the three-dimensional elastic-plastic behavior of polymer-based nonwovens. Starting from a representative volume element based on micro-computed tomography, we simulate and characterize the material's deformation when subjected to tension, compression, and shear loads in the machine direction (MD), cross direction (CD), and z-direction (ZD). The simulation results are validated using an extensive 3D material testing program. Finally, the dependency of the effective elastic-plastic deformation behavior on a limited number of selected microstructural parameters is discussed. This dependency forms the basis for the usage of digital twins to predict the deformation behavior of virtual microstructure designs.

KEYWORDS

Nonwovens, virtual filter media development, microstructural simulation, virtual testing lab.

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INTRODUCTION

Filtration is one of the most common methods to remove aerosol particles from a fluid, in which fibrous filter media captures the airborne particles. We focus on nonwoven filter media within the current research project, consisting of disordered fibers consolidated by chemical, thermal, or mechanical bonding into a semi-random fiber network. These nonwoven media serve in various applications, including cabin air or HVAC filtration applications. The following properties specify a filter's performance [1]:

1. Filtration efficiency, defined by the fraction of particles of a given size captured by the filter,
2. initial pressure drop, describing the resistance of the filter media and its energy efficiency,
3. dust holding capacity (DHC), describing the mass of dust captured until the filter reaches the clogging point. An indicator of the service life of a filter medium.

Especially for environmental filtration applications, for example, fine dust filtration, a minimal pressure drop is desired to minimize the carbon footprint and power consumption. Two materials are available, combining high filtration efficiency for fine particles with a low pressure drop in high volume flows. These materials are either fiberglass-based or polymer-based. However, fiberglass-based materials have two disadvantages compared to polymeric fiber materials. After use, fiberglass materials are considered hazardous waste. Also, breathable fragments of the fiber microstructure can break off and pass into the filtered air. On the other hand, polymer-based materials can carry an electrostatic charge to improve filtration efficiency further. Polymer-based materials also allow comparable easy manipulation of microstructural parameters in the filter media manufacturing process.

Filtration simulations employing parameter optimizations improve the filter media's filtration performance by manipulating their microstructural properties [2]. This method leads to microstructural designs with optimized filtration quality parameters. However, the new materials' effective mechanical properties are undetermined in the microstructural design process at this point. To assess the feasibility of new microstructural designs for selected filtration applications and for further processing in the established manufacturing process, the ability to predict the effective mechanical properties of a microstructural design is crucial. Therefore, this study investigates the characteristic deformation behavior of synthetic nonwoven filter media and aims to develop a microstructural simulation model capable of describing the elastic-plastic deformation behavior of polymer-based nonwovens.

STATE-OF-THE-ART

Nonwoven materials exhibit a complex and anisotropic deformation behavior. Past works have considered nonwovens mainly as a 2D material [3, 4, 5]. Nevertheless, Stenberg concluded that for paper-like materials in conversion processes like calendering, folding, cutting, and creasing, the consideration of through-thickness material properties is essential [6, 7]. These conversion processes are very similar to calendering, embossing, and pleating, which are part of the filter elements' rotative manufacturing process (compare Fig. 2). Therefore, the consideration of out-of-plane deformation creates the need for a 3D microstructural simulation model capable of describing the highly anisotropic material behavior of nonwovens.

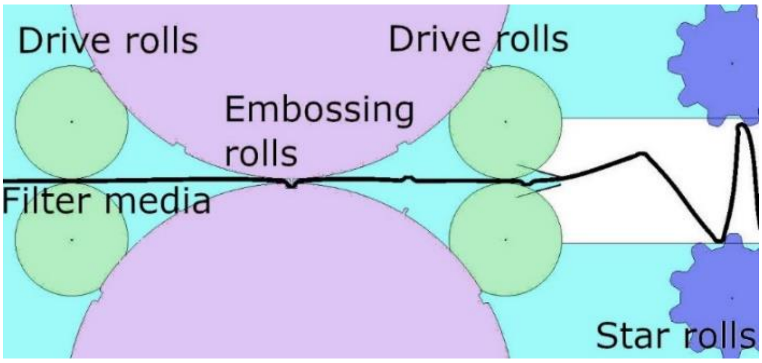

Fig. 2: Simplified schematic of the rotative manufacturing process of pleated filter elements.

Relevant 3D microstructural simulation models of nonwoven structures are still scarce [8]. The requirement of minimum domain size, to include enough of the microstructural parameters' statistical distributions to gain a representative volume element (RVE), paired with a minimum resolution requirement, to achieve a sufficient resolution of the stress gradients, make these investigations computationally challenging. Liu [8, 9] developed a 3D finite element analysis (FEA) based on micro-computed tomography scans (µCT-scans) for the analysis of nonwoven structures. The load cases of tension and compression in the three spatial directions have been simulated. The mentioned model discretizes fibers and bond points as straight beam elements and applies the basic beam assumption. Due to the simplified implementation of fiber contacts as spring elements, the model can only account for densification in a limited capacity. It also neglects fiber flexures. Therefore, it can only account for nonlinear fiber deformations (e.g., fiber buckling) within a limited scope. The model's viability for more complex multidirectional load cases, like shear, has not been shown. However, these load cases greatly influence the result of the conversion processes, as they are part of the rotative manufacturing process and, thus, are of particular interest. The authors mention the computational challenges of direct 3D FEA simulations on µCT-scans and apply their simplified model to balance structural considerations and computational efficiency [9]. While µCT-scans are very suited to account for the microstructural properties [10], the discretization using straight beam elements leads to a high preprocessing workload. The necessary preprocessing effort makes industrial applications on a larger scale challenging. Therefore, a more generalized 3D microstructural simulation model for tension, compression, and shear load cases is required, capable of running directly and computationally efficient on high-resolution µCT-scans.

PROBLEM AND OBJECTIVE

Describing the 3D deformation behavior of fibrous and porous filter media using a microstructural simulation model is a complex task. The scope of this work makes the description of the fiber material with elastic-plastic material laws necessary. Furthermore, simulating the three principal load cases of tension, compression, and shear in 3D with fitting boundary conditions is a prerequisite for this work. Fiber bending and fiber buckling in the load cases of compression in-plane, tension out-of-plane, and shear out-of-plane demand for the consideration of nonlinear geometric behavior. Another challenge are the size/resolution requirements of the domain and the corresponding calculation times.

The microstructural discretization's resolution should allow for a minimum of five to six voxels/integration points over the fiber's diameter to account for stress gradients over the fiber cross-section. Throughout this investigation, an RVE convergence study showed that a minimum domain size of 1.2 mm side length is necessary for the nonwoven investigated in this work to represent the mechanical behavior on the continuum level. However, this value is not universally valid, and a convergence study has to be performed if the minimum representative domain size is in doubt. The single-layer nonwoven filter material has fibers made of polypropylene mono- and copolymer with diameters of approximately 22 µm and a material thickness of approximately 1 mm. This filigree structure, coupled with the required minimum domain size, leads to meshes with very high element counts. The minimum element count for the nonwoven researched in this work is around 4 million elements, and the maximum count is around half a billion elements. In principle, a standard FEA can be used to simulate nonwoven materials. However, the high number of elements makes this approach computationally costly.

The GeoDict-ElastoDict software package with the Feelmath-LD solver was used instead to address this problem and achieve calculation times feasible for industrial use. The solver is particularly well suited to calculate complex microstructures' effective material properties using µCT-scans [11]. Compared to an FEA solver, this calculation scheme achieves much shorter calculation times on µCT-scans with high resolutions.

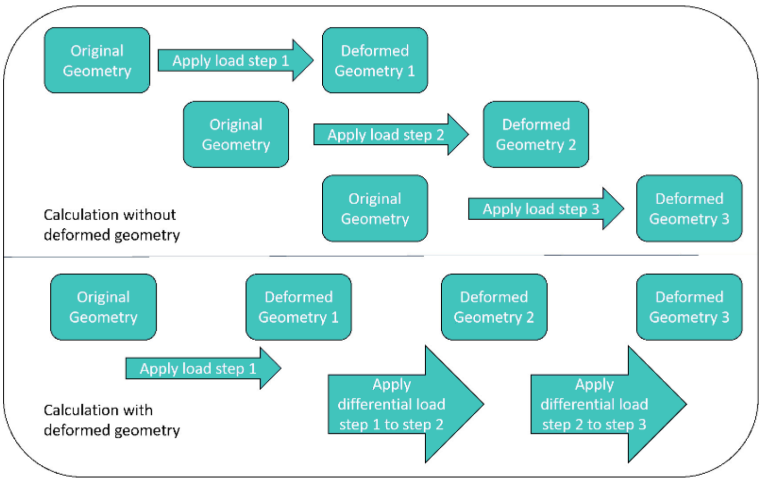

Fig. 3: Principle sequence of calculations with and without deformed geometries. Figure based on [12].

Feelmath-LD offers the choice of multiple material models for the user, including elastic-plastic material laws. Accounting for plasticity was a requirement since this investigation is motivated by developing a two-scale process simulation model for the manufacturing of synthetic filter elements. To account for the geometric nonlinear material behavior observed in most load cases, ElastoDict can calculate on deformed geometries. After every physical time step, the resulting deformed microstructure is remeshed (defined as resampling in ElastoDict, compare [12]), and the new mesh serves as the initial deformation state for the next calculation step. Fig. 3 shows the principle sequences of the algorithms for calculations on deformed and undeformed structures.

SIMULATING THE MECHANICAL BEHAVIOR OF NONWOVEN MATERIAL IN 3D

A microstructural simulation model was developed to gain a better understanding of the relationship between fiber microstructures and the effective mechanical properties. The same microstructural simulations can be used in a homogenization calculation to predict the effective mechanical parameters for subsequent process simulations.

Testing and Preparation of the Simulation Model

At the beginning of this investigation, the characteristic 3D deformation behavior of the fibrous and porous material was unknown. Therefore, an extensive 3D material testing program was conducted, characterizing the deformation behavior under tension, compression, and shear loading in all three spatial directions. The results of these tests also served to validate the microstructural simulation model. The material tests took place at the Institute of Aerospace Engineering at the Technical University of Dresden. The complex nature of 3D testing thin samples of comparatively soft material made the usage of special testing equipment and sensors necessary. The optical strain sensor system GOM Aramis for digital image correlation measured the local strain fields in all tests conducted. Fig. 4a shows the testing rig for the short-span compression tests in-plane. The sample support prevents the test sample from compression buckling under the in-plane compression load.

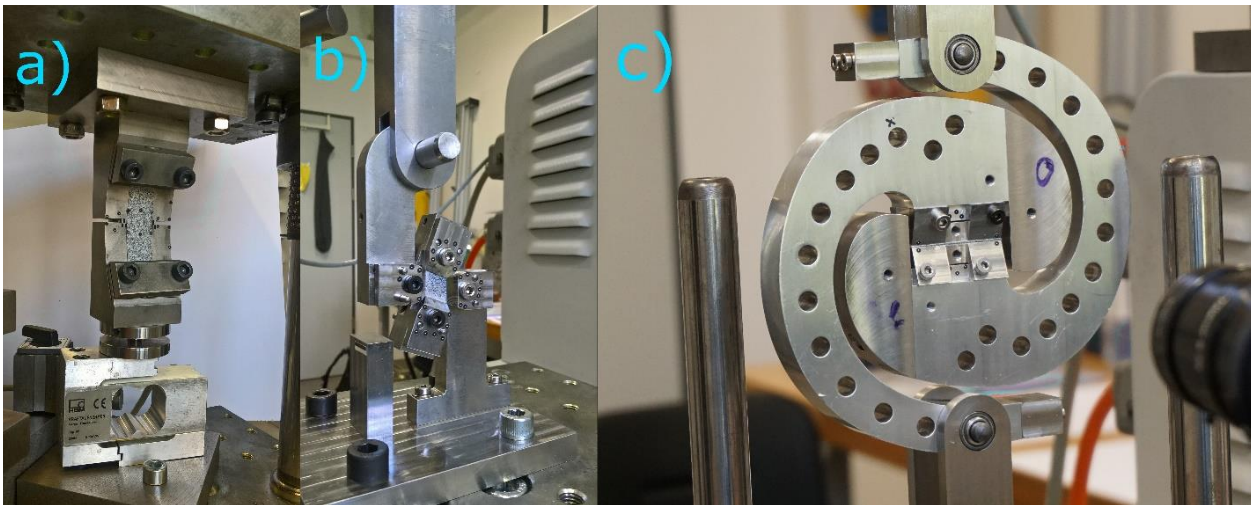

Fig. 4: Special testing equipment for the testing of thin samples of soft material (Source: ilr, University of Dresden).

Fig. 4b shows the shear frame redirecting the unidimensional tension load into a shear load in-plane. The ARCAN device shown in Fig. 4c redirects the unidimensional tension load into tension, compression, or shear load out-of-plane, depending on the attachment hole used on the device. These tests were initially designed for paper-like materials. However, they are also suited to characterize synthetic filter media's deformation behavior due to the two nonwoven materials' similar thin, fibrous and porous nature.

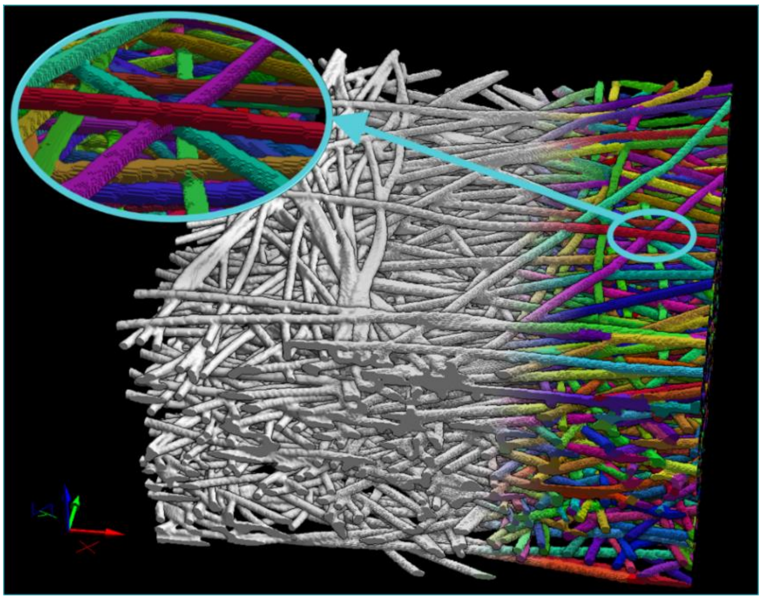

Fig. 5: Fiber structure segmented into equidistant voxel mesh with a resolution of two µm per voxel.

Microstructural investigations have been performed on a selected CAF filter material using scanning electron microscopy and µCT-scans. The µCT-scans were used to generate 3D high-resolution representations of the fiber microstructure (compare Fig. 5).

The effective material parameters for this fiber material slightly differ from the manufacturer's values for the bulk material. This change in effective material parameters originates from the nonwoven's spunbond manufacturing process. This process changes the crystallinity in the material, which in turn changes Young's modulus and yield stress. A Differential Scanning Calorimetry served to deduce the new crystallinity, and a correlation between crystallinity and Young's modulus/yield stress was used to calculate the new material parameters based on the work of Menyhárd et al. [13].

Microstructural Analysis and Digital Twin Modelling

As the Feelmath-LD solver implemented in GeoDict shows, the continuing development of fast simulation codes makes predicting the 3D elastic-plastic behavior for tension, compression, and shear practical. The virtual predictions can be sped up further by using digital twins with periodic material structures. Digital twins modeled with a periodic material structure allow for the usage of periodic boundary conditions in the calculation, which converge much faster against the solution than calculations with symmetric boundary conditions.

In the present work, microstructural simulations showed that dominant mechanical deformation behaviors of synthetic nonwovens on the continuum level depend on a limited amount of microstructural parameter distributions. Moreover, these classifiable microstructural properties exist even in nonwovens with their random fiber networks. Therefore, RVEs and digital twins can be modeled for this class of materials.

Average values for the solid volume fraction, fiber orientation distribution, fiber diameter distribution, and fiber curvature distribution have to be determined to create a digital twin.

GeoDict offers the module FiberFind to analyze these distributions. In this step, a microstructural analysis was performed using the µCT-scan shown in Fig. 5.

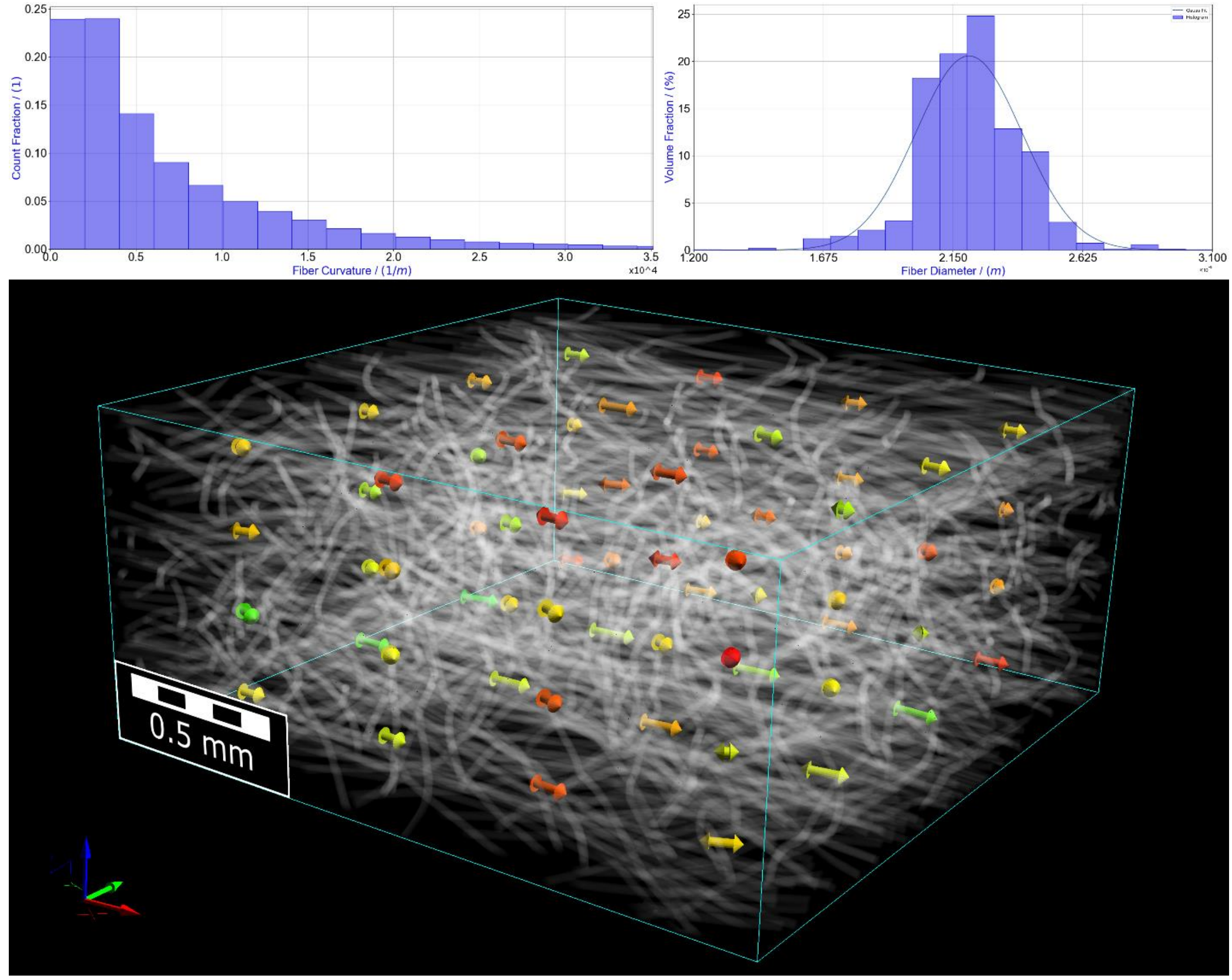

Fig. 6: Results of the microstructural analyses of the fiber curvature (top left), fiber diameter (top right), and fiber orientation distributions (bottom).

Fig. 6 shows the distributions of the microstructural parameters fiber curvature and fiber diameter. Also shown is the virtual representation of the local fiber orientation tensors in a 4x4x4 grid. These microstructural parameters were used to create a digital twin of the fiber network shown in Fig. 5. A digital twin represents the fiber structure with the same microstructural properties as the µCT-scan but consists of regular (fiber) elements. Fig. 7 shows the digital twin, which shows a more homogenous fiber network than the µCT-scan in Fig. 5 but has matching statistical properties regarding the described microstructural parameter distributions.

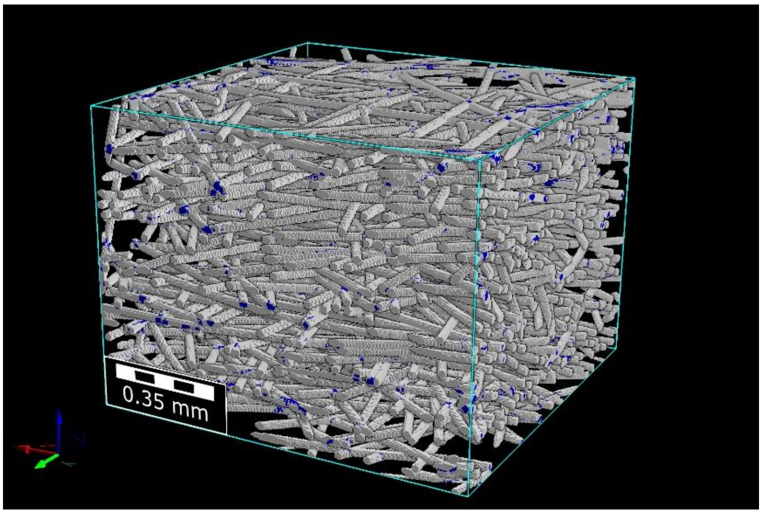

Fig. 7: Resulting fiber structure for the digital twin of the material sample shown in Fig. 5 with fiber overlap in blue.

Simulation and Discussion of Results

Microstructural simulations were performed based on an elastic-plastic material model. After an RVE convergence study, the necessary domain size for this material was defined at 1.2 mm side length. The minimum resolution for the following calculations was four micrometers per voxel. In-plane tension and out-of-plane compression simulations were performed on µCT-scans and digital twins to prove the viability of digital twins. Fig. 8 compares the simulation and test results.

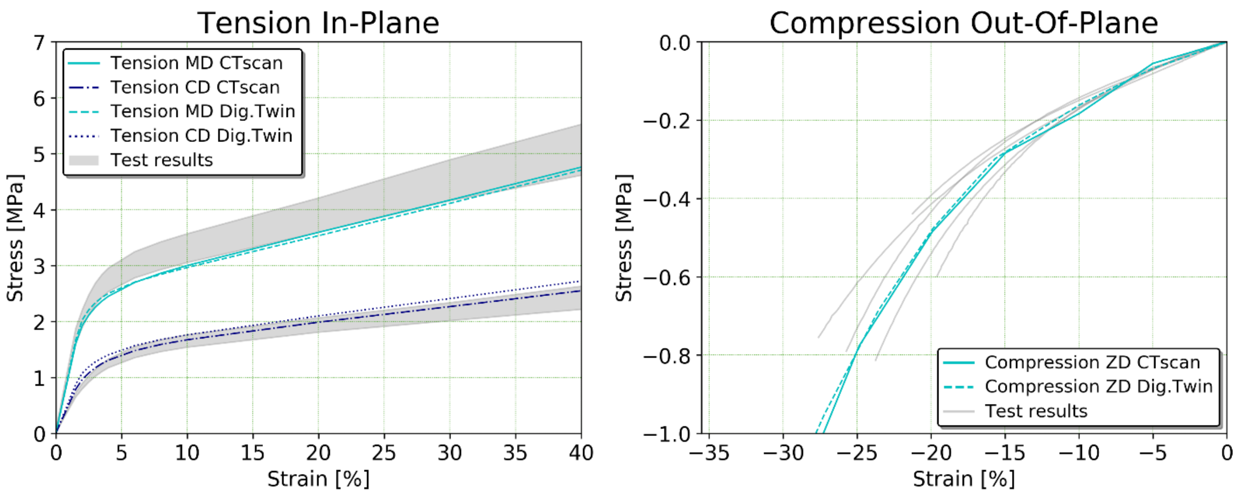

Fig. 8: Stress-strain curves of the microstructural simulations tension in-plane and compression out-of-plane.

The resulting stress-strain curves show only slight deviations between calculations on µCT-scans and digital twins. The results are corroborating the viability of digital twins for microstructural simulations. The results also show good accordance with the testing results (gray areas/curves), validating this calculation scheme for the simulation of nonwovens for the load cases tension in-plane and compression out-of-plane. These load cases are easy to test without special equipment and are therefore preferable as validation load cases for future material studies. The deformation behavior of the tension load case in-plane is primarily controlled by the tension deformation of fibers in or close to the load direction. Fibers transversal to the load direction have only a minor influence on the tension deformation behavior on the continuum level. The deformation behavior for the compression load case in ZD is controlled mainly by densification mechanisms, making the solid volume fraction the most influential parameter for this load case. The nonlinear fiber buckling under densification makes the calculation based on deformed geometries essential.

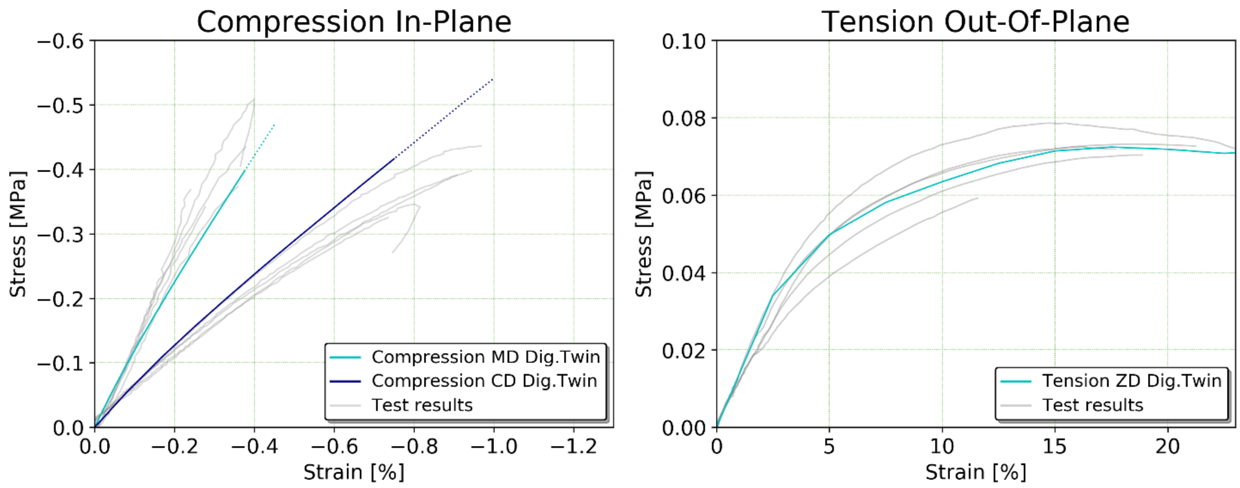

Fig. 9: Stress-strain curves of the microstructural simulations compression in-plane and tension out-of-plane.

Fig. 9 shows the resulting stress-strain curves of the compression simulation in-plane and the tension simulation out-of-plane. A simple maximum strain failure criterion has been applied to the simulation results for the load case compression in-plane. The stress-strain curves of the compression load case depict the results beyond the material failure as dotted lines. The deformation behavior in these load cases is defined mainly by fiber bending and fiber buckling. These nonlinear geometric deformations require the calculation based on deformed geometries for both load cases. The tension load case out-of-plane vividly shows the softening of the material. After reaching a maximum stress value, material damage in the bond points causes a decrease in the material's ability to resist deformation. While the material model cannot directly account for material failure (softening), it correctly predicts the material behavior up to the maximum stress.

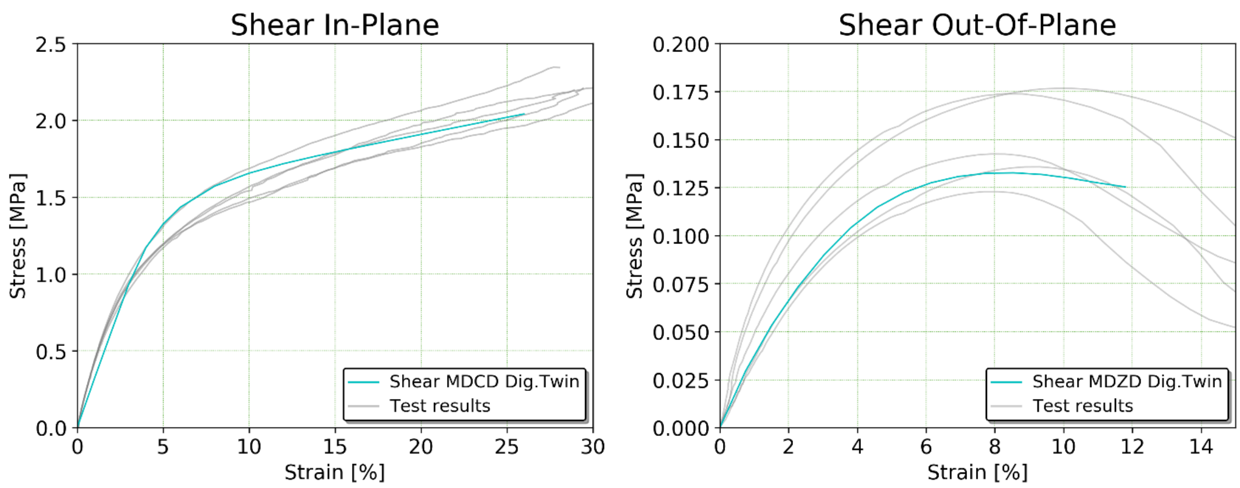

Fig. 10: Stress-strain curves of the microstructural simulations shear in-plane and shear out-of-plane.

Fig. 10 shows the resulting stress-strain curves for the shear load cases. The deformation behavior for the load case shear out-of-plane resembles the tension in the ZD load case's behavior. The fibers are mainly subjected to fiber bending, and after reaching maximum stress, the material is experiencing material softening. The large nonlinear geometric deformations make the calculation based on deformed geometries necessary for this load case. The calculation without deformed geometries for the load case shear in-plane shows minor deviations from the test results. The results underestimate the stiffness in the elastic range and hardening in the plastic range. However, the deviations stay within acceptable limits. Like the tension in-plane load case, fibers concurrent with the load direction are strained and carry the load. In distinction to the uniaxial load in the tension in-plane load cases, the load in the load case shear out-of-plane is biaxial in ±45° direction.

CONCLUSION

The existence of RVEs for this type of material could be corroborated within this work. Furthermore, the model can predict the nonwoven material's elastic-plastic behavior for tension, compression, and shear load cases in three spatial directions.

Additionally, the viability of digital twins for the fiber structure's mechanical simulation could be demonstrated, showing that the mechanical behavior depends primarily on a small number of microstructural property distributions. The usage of digital twins enables the prediction of effective mechanical behaviors of virtual prototypes depending on their microstructural parameter distributions. Parameter studies should offer further insight into the nonwoven's effective mechanical parameters on the continuum level and their direct dependence on the microstructural properties. Further investigations into this interaction is necessary and planned, hopefully allowing the future integration of mechanical requirements into the modeling process of virtual filtration designs before prototyping.

A better understanding of the micro-mechanisms of deformation under the varying principle load cases has been gained. This improved understanding can be used to provide a more realistic description of the deformation behavior for selected load cases observed in the application or manufacturing of filter elements.

The microstructural simulation model demonstrated its suitability for homogenization calculations and the prediction of the effective mechanical parameters of virtual filter designs. It is planned to use these parameters in manufacturing process simulations currently under development, effectively creating a two-scaled process simulation model that predicts the virtual designs' viability for the rotative manufacturing process.

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