

## Stochastic 4D modeling of fiber-based materials for varying degrees of compression

Gerd Gaiselmann<sup>a</sup>, Christian Tötzke<sup>b</sup>, Ingo Manke<sup>b</sup>,  
Werner Lehnert<sup>c</sup>, Volker Schmidt<sup>a</sup><sup>a</sup>Universität Ulm, 89069 Ulm, Germany<sup>b</sup>Helmholtz-Zentrum Berlin für Materialien und Energy,  
14109 Berlin, Germany<sup>c</sup>Forschungszentrum Jülich, 52428 Jülich, Germany

The morphological micro-structure of complex porous materials is closely related to their physical properties, in particular with transport processes of gases and fluids. Thus, the systematic development of 'designed' morphologies with improved physical properties is an important task.

Mathematical models from stochastic geometry can help to solve this problem, since they can be used to provide a detailed, quantitative description of complex microstructures in existing materials.

More precisely, in order to enhance the understanding of the various physical processes within the GDL, stochastic microstructure models have been developed which are fully parameterized, see e.g. [1, 2, 3, 4]. By systematic modifications of model parameters in combination with numerical transportation models, virtual 3D morphologies and virtual transportation processes in these morphologies can be simulated. In this way, it is possible to elucidate the correlation between the microstructure of the GDL and its physical properties and thereby to detect optimized morphologies.

In this talk, we present a parameterized stochastic model which describes the micro-structure of (strongly) curved fiber-based materials under varying degrees of compression.

Thereby, the uncompressed material is described by a stochastic model for fiber-based materials introduced in [2]. The general idea for the 4D compression model is to assume that the fibers are only translated in z-direction (i.e. direction of compression). Subsequently, given a degree of compression  $d \in [0, 1]$ , a function  $c_d$  manages the size of translation of fibers in z-direction where the translation depends on the location of the fiber within the material.

Furthermore, the 4D compression model distinguishes between two different kinds of compression.

The first kind compresses the material with a flat stamp (Figure 1), where the second one uses a stamp with a channel-bar profile (Figure 2).

Additionally, a method is proposed to adequately estimate the translation function  $c_d$  from experimental data.

As an example of application, the compression model is used for a specific non-woven gas diffusion layer (GDL) in polymer membrane fuel cells.

Finally, the 4D compression model is validated by comparing several structural characteristics computed for a sequence of 3D X-ray synchrotron data (Figure 1 and 2) with varying degrees of compression [5] and for realizations of the compression model, where an excellent agreement of experimental and virtual data has been found.

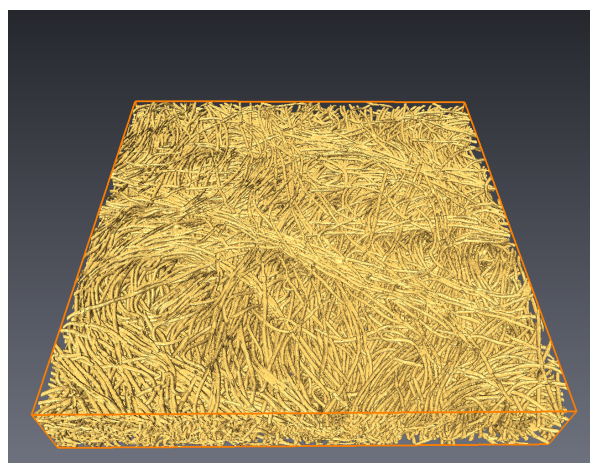


Figure 1: Perspective view on a compressed GDL sample (Freudenberg H2315) illustrating the compression by a flat stamp.

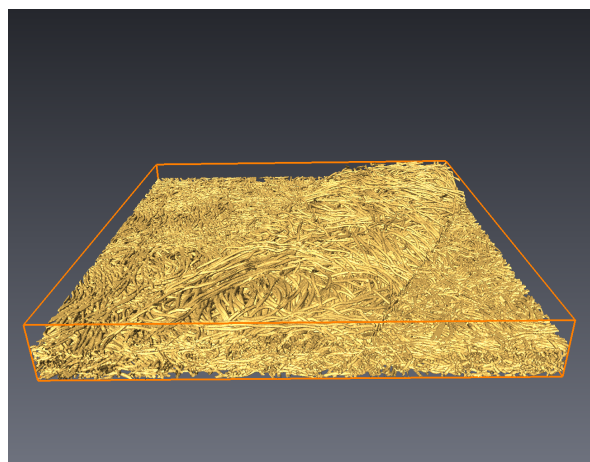


Figure 2: Perspective view on a compressed GDL sample (Freudenberg H2315) illustrating the compression by a stamp with channel-bar profile.

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[4] Schulz, V.P., Becker, J., Wiegmann, A., Mukherjee, P.P. and Wang, C.Y. (2007). Modeling of two-phase behavior in the gas diffusion medium of PEFCs via full morphology approach. *Journal of the Electrochemical Society*, 154, B419-B426.

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