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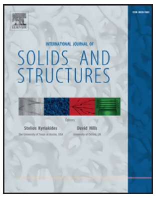

Thermal fiber orientation tensors for digital paper physics

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ABSTRACT

We estimate the orientation of wood fibers in porous networks like paper, paperboard or fiberboard by computing digital thermal conductivity experiments on micro-computed tomography (μCT) images with artificial isotropic thermal conductivity parameters.

The accuracy of mechanical and thermal constitutive models for porous wood fiber based materials crucially depends on knowing the wood fiber orientation. Unfortunately, due to the high porosity, the micro-heterogeneity of wood fibers, the high carbon content of organic materials and the unknown additives present in industrial paper, μCT-scans often exhibit low contrast and strong artifacts. Conventional image processing approaches encounter difficulties, as they rely upon convex fiber cross sections.

We propose a solution by circumventing the segmentation of single wood fibers in μCT images, by performing thermal conductivity simulations on binarized wood fiber structures, where an artificial isotropic thermal conductivity is associated to the fibers and the pore space is considered as isolating. The local and global temperature fluxes are assembled into a fiber orientation tensor. This method overcomes the limitations of the mentioned local image processing approaches, as individual fibers need not be resolved and convergence for increasing resolution is a consequence of abstract mathematical theory.

We use our novel method to analyze large three-dimensional μCT-scans and a synchrotron scan of a paperboard sample, serving as the starting point of an accurate micromechanical modeling of the effective anisotropic mechanical behavior of paper and paperboard. These results are crucial for calculating the mechanical strength of deep-drawn paperboard, which will be accomplished in a subsequent article.

1. Introduction

Due to online trading packaging materials for food industries face novel challenges. In addition to resource efficiency these materials require high mechanical stability necessary for the transport. These considerations give impetus for understanding the characteristics and the mechanical behavior of wood fiber based materials like paper, paperboard or fiberboards.

This work is motivated by quality considerations of paperboard forming (Wallmeier et al., 2015a) utilized in the packaging industry. For the deep-drawing process we consider, which is described in detail in Hauptmann and Majschak (2011), a flat sheet is deep-drawn to form the final geometry, see Fig. 1. In contrast to polymer materials the material extensibility of paperboard is much lower (Hauptmann and Majschak, 2011; Vishtal and Retulainen, 2012) and achieving a visually appealing appearance, in particular a flat surface, is much more challenging due to wrinkling, see Fig. 2, which is caused by the material properties of paperboard.

The formation of wrinkles depends strongly on the process conditions like the forming speed and forming temperature. To ensure high quality for production in quantity, an accurate finite element modeling of the deep-drawing process is required. Previous work (Wallmeier et al., 2015b) showed an excellent agreement of the simulation with experiments up to the point where wrinkling dominates.

The mechanical behavior of paperboard exhibits anisotropic elastic and inelastic properties (Xia et al., 2002) which additionally depend on humidity and temperature, and raises challenges for the accurate modeling (Linvill and Östlund, 2014). The reason for the formation of wrinkles is to be found in the microscopic fiber network structure of paperboard (Ostoja-Starzewski and Stahl, 2000). To gain insight into the effects of highest order, a

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Fig. 1. Geometry of the deep-drawn paperboard in use for new packaging applicationswith a diameter of 100 mm and a height of 25 mm, cf. Hauptmann and Majschak (2011).

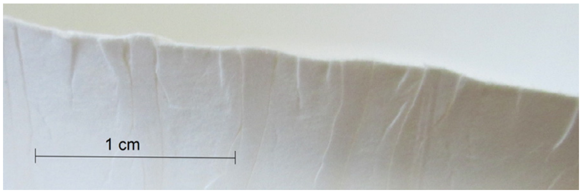

Fig. 2. Close-up view on ears and wrinkles at the top of the rim for a specimen with unfavorable processing conditions.

microstructural characterization of the material before and after the deep-drawing process is necessary.

In addition to the degree of porosity and its local variation the wood fibers'orientation represents the quantity of primary interest, again prior and after deep-drawing, as this orientation determines mechanical properties like strength and stiffness of wood fiber based materials (Sliseris et al., 2014).

Conventional image processing algorithms (Altendorf and Jeulin, 2011; Gadala-Maria and Parsi, 1993; Vahlund and Gebart, 2001), see (Wirjadi et al., 2004) for a recent overview, expect the fibers'cross section to be almost circular, in particular at least convex, to obtain a local fiber orientation which is subsequently averaged and gathered into a global fiber orientation tensor. This approach is extremely successful for short fiber reinforced plastics, relying upon the cylindrical structure of the fiber reinforcements.

For natural fibers, like wood fibers, these algorithms encounter problems. First and foremost, the geometry of the fiber is challenging: in cross section wood fibers have the shape of thickened ellipses, but the thickness and orientation of these ellipses may vary strongly along the fiber's length. Secondly, micro-computed tomography (μ-CT) scans of the microstructures of wood fiber based materials suffer from low contrast and strong artifacts due to the high carbon content of organic materials and the oftentimes unknown additives involved.

For the work at hand, an additional complication arises: during the forming process, the wood fibers undergo irreversible mechanical deformation, leading to fiber breakage or partial collapsing. These effects are visualized in Fig. 3. A synchrotron X-ray tomographic microscopy scan with $0.32\mu m$ resolution was conducted on a deformed paperboard sample. For undeformed paperboard, fibers primarily exhibit a planar orientation in the $x-y$-plane and are further stacked in the z-direction.[1] During the deep-drawing process these stackings are folded, see Fig. 3 (left). Furthermore, there are visible gaps between these stacks.

Fig. 3 (right) depicts a slice in z-direction of the associated binarized high resolution voxel image. Discerning individual fibers appears challenging. We tried to identify an individual fiber in Fig. 3 (right), highlighted in red. The fiber is strongly malformed: the lumen no longer pervades the length of the fiber, but is compressed at times, and the fiber's wall also exhibits vacancies. In particular, associating a fiber orientation to this single fiber by a local image processing technique is difficult.

To resolve these complications we propose to use digital thermal conductivity experiments on the voxel images obtained from micro-tomography to associate local and global fiber orientation tensors. We associate an isotropic thermal conductivity to the fibers, which is devoid of any physical meaning, and compute the effective thermal conductivity tensor L^{eff}. Normalizing (and undimensionalizing) this tensor to have trace 1 leads to an orientation tensor A^{ThOr}, which we call thermal orientation tensor (ThOr). This tensor has a number of positive features:

1. A^{ThOr} is independent of the isotropic thermal conductivity we started out with.
2. A^{ThOr} is a symmetric and positive definite 3×3-tensor. In particular, an eigenvalue decomposition of this tensor sheds light upon the principal orientation axes of the specimen, and the relative distribution of fibers in these directions.
3. A^{ThOr} can be computed by different discretization methods, like finite element (Yu et al., 2015), finite difference (Willot et al., 2014) or spectral methods (Eyre and Milton, 1999). However, for increasing the number of degrees of freedom, all of these methods converge to the same thermal fiber orientation tensor A^{ThOr}. In particular, the numerical method for obtaining A^{ThOr} is secondary. Additionally, the A^{ThOr} tensors for different resolutions can be compared directly, in contrast to most conventional image processing techniques, where the filter bandwith or the window size has to be calibrated to the resolution.
4. It is possible to define a local thermal conductivity tensor, depending on the microscopic base point, which recovers the effective global thermal conductivity in the mean. This can be considered as a consistency condition. Using the identical normalization gives rise to local thermal fiber orientation tensors which are again independent of the isotropic thermal conductivity used for the simulation.

This work is organized as follows. After exposing the fundamentals of thermal conductivity homogenization in Section 2 we briefly describe the FFT-based homogenization technique for thermal conductivity in Section 3, which permits a rapid and memory-efficient evaluation of L^{eff} and $L^{loc}(x)$ on voxel grids. The critical properties of the thermal fiber orientation tensors are deduced in Section 4, culminating in a detailed fiber orientation analysis of paperboard before and after the deep-drawing process on large μCT and synchrotron scans in Section 5.

2. On the homogenization of thermal conductivity

We consider a rectangular box $Y=[0,L_1]\times[0,L_2]\times[0,L_3]$, occupied by a solid $\Omega\subseteq Y$. For the application at hand, the binarized microstructure determines a decomposition of Y into a solid Ω and a porous part $Y\backslash\Omega$, see Fig. 4. Fix a scalar thermal conductivity k, and solve, for the three cases $i=1,2,3$, the thermal conductivity equation according to Fourier's law

$$\operatorname{div} q_i = 0, \quad q_i = -k(e_i+\nabla T_i) \quad \text{in} \quad \Omega \tag{2.1}$$

with periodic boundary conditions

$$T_i(x+L_j e_j) = T_i(x) \quad \text{for all} \quad x\in Y \quad \text{and} \quad j = 1,2,3,$$

and the insulation boundary condition $n\cdot q_i = 0$ on the interface $\partial\Omega$.

Here, e_i denotes the unit vector in the i-th coordinate direction, T_i is the local temperature field on Ω, ∇T_i is the temperature gradient, q_i denotes the temperature flux and n denotes the

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[1] Throughout this article, we associate the x-direction with the machine direction (MD) and the y-direction with the cross direction (CD) of paperboard.

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