MULTISCALE MODELING OF PAPER

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Abstract
Laminated paperboard is widely used in packaging products. It is generally composed of several pulp fiber layers bonded to each other by starch or adhesive material, leading to macro anisotropic elastic-plastic behavior. The aim of this study is to predict the mechanical properties of a paper layer by using a three-scale approach consisting of the fiber wall scale, the fiber network scale, and the layer scale. The homogenization was first performed on the fiber wall scale, where the fibrils were considered at some orientation embedded in a polymeric matrix. The obtained homogenized response was then input to the single fibers in the network model, which was the second scale considered. At this level, the virtual microstructure was generated first by creating the individual fibers in different layers, and then by simulations of artificial compression to obtain the practical fiber volume fraction. Thereafter, the interaction between fibers was described by interface-based cohesive zone model introduced in all fiber-fiber contact areas. Finally, the macroscopic mechanical properties were obtained by applying periodic boundary conditions and subsequent numerical homogenization was performed on the generated fiber network.

1. Introduction

Laminated paperboard is widely used in packaging products. Depending on the specific requirement, it can be easily designed as a single layer paper or multi-layer sandwich structure. The manufacturing process of paper sheet consists of turbulent flow of a suspension of wood fibers in water, its filtration and sedimentation on a wire mesh and further mechanical/chemical treatment. Therefore, paper is generally composed of several pulp fiber layers bonded to each other by starch or adhesive material. Its mechanical properties are strongly controlled by single fiber properties and inter-fiber bonds. In addition, the stochastic nature of the drainage process leads to a planar network structure with more fibers along the machine direction (MD). As a result, this material exhibits a highly anisotropic mechanical behavior, including anisotropic elasticity, initial yielding, strain hardening, and tensile failure.

Paper typically has three scales of importance: the fiber scale, the network scale, and the paper layer scale. Due to the importance of paper products in packaging and printing industry, there are lots of studies on the paper layer or laminated paperboard, see e.g. Nygårds et al. [1], Bolzon and Talassi [2], Wallmeier et al. [3]. These studies have been conducted to analyze paper layer deformation during creasing, folding and deep drawing using continuum based models. More recently, some other

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methods have been developed to predict the influence of moisture [4] and deformation rate on paper's mechanical properties [5].

The study of network modeling is still limited and underdeveloped because of the complex nextwork structure. It is important to develop such models for several reasons. One is to understand how the single fibers and inter-fiber bonds affect the macro mechanical properties. In particular, the network simulation enables the investigation of the deformation mechanism behind the nonlinear phenomena observed in experiments. Additionally, the fiber orientation, length and diameter distributions often have a profound effect on the macro properties, which can also be studied using network modeling. Finally, it enables the prediction of material parameters for the continuum based model. These parameters are usually difficult to obtain experimentally for a thin paper layer. In the literature, most network models have too many simplifications to be able to capture local events like cross-sectional shapes and frictional slippage. Such models utilize either a rigid-bond assumption (see [6] for a systematic review) or treat the fiber segments as beam elements [7-9]. Recent models have attempted to include the inter-fiber bond deformability [10].

At the fiber level, the single fibers are actually composite materials themselves, since the cell wall of pulp fibers consists of a layered structure of cellulose micro-fibrils embedded in a lignin and hemicellulose matrix. The micro-fibrils are around the axis of the fiber and form a helical assembly in the bundles. The fibril orientation angle governs the mechanical properties of the fiber, as shown in [11]. Recently, a 3D finite-element model that accounts for the presence of micro-fibrils has been developed to study the fiber cyclic loading behavior [12]. Similar models have been used in other studies focusing on either the elastic properties of the fiber [13] or the bond properties [14, 15].

In order to predict the macro mechanical properties of paper, a three-scale approach was adopted, with focus on the two lower scales in this work. The following section of this study outlines the general model framework, along with the implementation of a homogenization and modeling strategy at different scales. This model provides the framework for determining the effect of microstructural parameters like fiber orientation, length, and inter-fiber bond on network behavior.

2. Modeling framework

Mechanical properties of a paper layer are highly dependent on its network architecture, such as the fiber orientation distribution, fiber length and diameter. A single fiber is actually a layered structure itself, with its mechanical properties dominated by the micro-fibril angle (MFA). Generally, the lower scale architecture has much lower length scales than the upper scale characteristic structure. Therefore, a three-scale algorithm was used to evaluate the effect of the micro architecture on macro material behavior in this study. Figure 1 shows the paper morphology at different scales and the corresponding representative volume element (RVE). The homogenization was performed first on the fiber wall scale, where the fibrils were considered at some orientation embedded in a polymeric matrix. The homogenized response was used to characterize single fibers in the network model, which was the second scale considered. At this level, the analysis was conducted on the generated virtual network. The homogenized stress-strain curves could then be used in macroscale modeling. In this workflow, a hierarchical approach was used, thus different scales were simulated and material parameters were passed from lower to upper scales. Hence it required the definition of material models on each length scale, which will be addressed later.

2.1. Single fiber scale

The original wood fiber typically consists of four major layers: the primary wall and three secondary layers S_1, S_2, and S_3. The secondary layers are composed of cellulosic micro-fibrils and a relatively compliant polymeric substance, comprising of hemicellulose and lignin, which is often treated as a matrix. Since the pulping process removes some contents of the surface layers, the thickest S_2 layer is assumed to dominate the mechanical behavior the fiber. Thereby, the fiber's structural stiffness can

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mainly be characterized by the properties and the amount of cellulose micro-fibrils embedded in a polymeric matrix of the S_2 layer, as well as their orientation along the fiber. In this study, the fiber was assumed to be purely elastic, because the measured force to break the inter-fiber bond was much smaller than the force for the fiber to achieve nonlinear deformation. In addition, several studies have found the dependence of MFA change on the fiber axial strain, and this will result in a stiffening effect in the case of fiber tension. However, the degree of stiffening is significantly small for high initial MFA, and the measured elastic modulus is not sensitive to the MFA change in experiments [16]. Hence, the MFA was assumed to be constant in the current study.

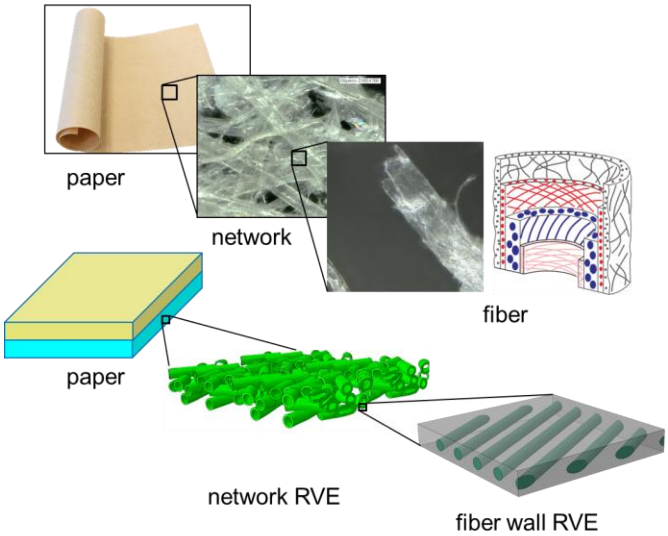

Figure 1. Comparison of the multi-scale nature of paper and the multi-scale framework for simulation.

Since the fiber wall was a composite reinforced with transversely isotropic micro-fibrils, the analytical micromechanical model developed by Chamis [17] was adopted to achieve the homogenized stiffness with sufficient accuracy. Using the material parameters taken from [12], Fig. 2 shows the dependence of the fiber axial Young's modulus on MFA with a micro-fibril volume fraction of 45%. It is clear that the effect of MFA is small enough to be neglected reasonably for higher MFA values.

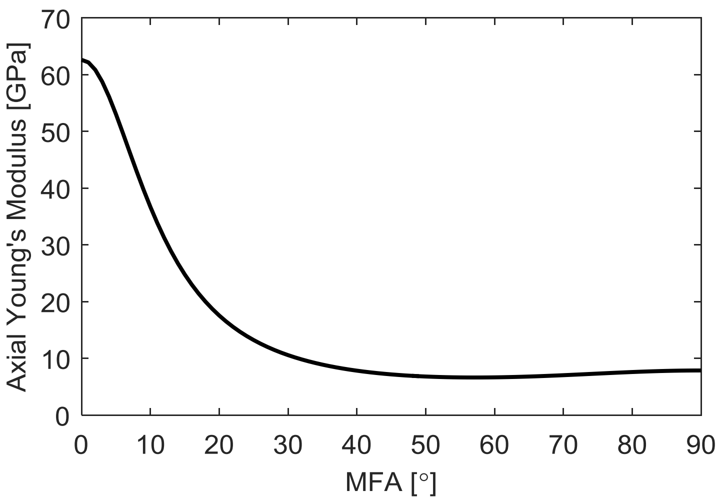

Figure 2. The effect of MFA on the fiber axial Young's modulus.

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2.1. Network scale

In order to perform analysis at the network level, the first step is to generate a network RVE large enough to represent the actual behavior of the microstructure. Using the experimentally obtained fiber length, diameter and orientation distribution, the periodic RVE was constructed in the following procedure. First, individual fibers were generated with input statistical distributions in different layers. Then, the fibers were brought into contact and deformed by an artificial compression loading in order to obtain realistic values for the fiber volume fraction. It should be noted that the periodic geometry was maintained by applying appropriate boundary conditions. Finally, the interaction between fibers was described by interface-based cohesive zone elements introduced at all fiber-fiber contact areas. Fig. 3 shows an example of a network RVE with 25 fibers.

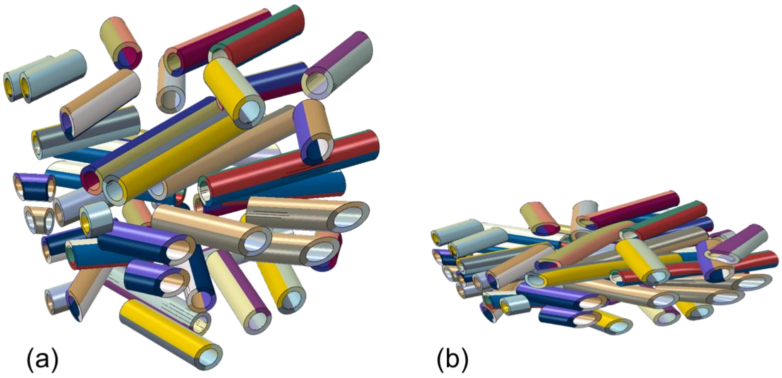

Figure 3. An example of fiber network RVE: (a) before compression (b) after compression.

To achieve the macro mechanical properties, six simulations, corresponding to uniaxial loading and pure shear loading states, were performed using periodic boundary conditions. The homogenized stress was calculated using

$$\bar{\sigma}_i = \int_v \sigma_i \mathrm{d}v \Big/ \int_v \mathrm{d}v \,, \quad (1)$$

where v is the RVE volume and i is the component of the stress vector in Voigt notation. In this way, the stress-strain curves can be obtained to compare with experimental results.

The network scale analysis allows simulating the RVE with various fiber structure and orientation. Therefore, it is possible to evaluate the influence of fiber length, diameter and distribution on the macro mechanical properties of paper. Additionally,

3. Conclusions

This study presented a three-scale approach to predict the mechanical properties of paper. Using this approach, the effect of MFA on fiber properties at the single fiber scale and the effect of the statistical fiber distribution on paper macro properties at the network scale can be evaluated. Furthermore, it is also possible to study the role of inter-fiber bonds in the network deformation. Consequently, the current study established a framework to study the fiber property and pass the information to the upper scale for fiber network analysis.

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References

[1] M. Nygards, M. Just, and J. Tryding, Experimental and numerical studies of creasing of paperboard. *International Journal of Solids and Structures*, 2009. **46**(11-12): p. 2493-2505.

[2] G. Bolzon and M. Talassi, A combined experimental and numerical study of the behaviour of paperboard composites up to failure. *Composites Part B-Engineering*, 2014. **66**: p. 358-367.

[3] M. Wallmeier et al., Explicit FEM analysis of the deep drawing of paperboard. *Mechanics of Materials*, 2015. **89**: p. 202-215.

[4] A.L. Erkkila et al., Hygro-elasto-plastic model for planar orthotropic material. *International Journal of Solids and Structures*, 2015. **62**: p. 66-80.

[5] D.D. Tjahjanto, O. Girlanda, and S. Östlund, Anisotropic viscoelastic–viscoplastic continuum model for high-density cellulose-based materials. *Journal of the Mechanics and Physics of Solids*, 2015. **84**: p. 1-20.

[6] R.C. Picu, Mechanics of random fiber networks-a review. *Soft Matter*, 2011. **7**(15): p. 6768-6785.

[7] J.X. Liu et al., Elasto-plastic analysis of influences of bond deformability on the mechanical behavior of fiber networks. *Theoretical and Applied Fracture Mechanics*, 2011. **55**(2): p. 131-139.

[8] A. Kulachenko and T. Uesaka, Direct simulations of fiber network deformation and failure. *Mechanics of Materials*, 2012. **51**: p. 1-14.

[9] C.A. Bronkhorst, Modelling paper as a two-dimensional elastic-plastic stochastic network. *International Journal of Solids and Structures*, 2003. **40**(20): p. 5441-5454.

[10] J. Sliseris et al., Numerical prediction of the stiffness and strength of medium density fiberboards. *Mechanics of Materials*, 2014. **79**(0): p. 73-84.

[11] I. Burgert and P. Fratzl, Plants control the properties and actuation of their organs through the orientation of cellulose fibrils in their cell walls. *Integrative and Comparative Biology*, 2009. **49**(1): p. 69-79.

[12] S. Borodulina, A. Kulachenko, and D.D. Tjahjanto, Constitutive modeling of a paper fiber in cyclic loading applications. *Computational Materials Science*, 2015. **110**: p. 227-240.

[13] R.C. Neagu and E.K. Gamstedt, Modelling of effects of ultrastructural morphology on the hygroelastic properties of wood fibres. *Journal of Materials Science*, 2007. **42**(24): p. 10254-10274.

[14] M.S. Magnusson and S. Östlund, Numerical evaluation of interfibre joint strength measurements in terms of three-dimensional resultant forces and moments. *Cellulose*, 2013. **20**(4): p. 1691-1710.

[15] A. Torgnysdotter et al., Fiber/fiber crosses: finite element modeling and comparison with experiment. *Journal of composite materials*, 2007. **41**(13): p. 1603-1618.

[16] I. Burgert et al., Microtensile testing of wood fibers combined with video extensometry for efficient strain detection. *Holzforschung*, 2003. **57**(6): p. 661-664.

[17] C.C. Chamis, Mechanics of composite materials: past, present, and future. *Journal of Composites, Technology and Research*, 1989. **11**(1): p. 3-14.

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