This is an author produced version of a paper published in Report #493, Department of Solid Mechanics, Royal Institute of Technology.

This paper has been peer-reviewed but does not include the final publisher proof-corrections or journal pagination.

Citation for the published Report:

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Report # 493, Department of Solid Mechanics, Royal Institute of Technology. (Trita-HFL. 0493)
Abstract
A periodic micromechanical modeling concept that utilizes continuum elements and a representative volume element (RVE) loaded with periodic boundary conditions is proposed to study paper network properties. The RVE has a volume of 1 mm³ and consists of fibers that are perfectly bonded. The fiber properties are represented by an isotropic elastic-plastic model that has an additional hardening effect at large strains, which has been observed for single fibers with high fibril angle. As non-linearities are accounted for in the material model, a fairly small number of elements are needed in the RVE to enable predictions of anisotropic fiber network properties, in this work 10×10×10 elements were used. The model has been used to simulate uniaxial tension tests in the three principal directions (MD, CD and ZD). An anisotropic fiber network structure was generated. With this structure, different deformation mechanisms were activated during loading in the different directions.

1. Introduction
Paper consists of pulp fibers bonded together in a network. Pulp fibers have a long and slender structure, where the length is in the interval 1-5 mm and the fiber width and height is in the interval 0.005-0.05 mm (Niskanen, 1998). Due to the processing history from wood to pulp, the fibers have gone through an extensive deformation and damage history before they are bonded into the paper fiber network. Paper materials are formed when the fibers bond to each other as water is removed and the fibers are dried. This generates a network where each fiber have typically 20-30 bonded segments.

The mechanical behavior of paper is controlled by the fiber properties and the bond properties. However, properties, such as stress-strain behavior and strength vary greatly between different fibers and bonds. In the literature variations of single fiber properties have been characterized with respect to: microfibril angle (Page et al., 1977; Page and El-Hosseiny, 1983; Sedighi-Gilani and Navi, 2007), defects (Jentzen, 1964; Kim et al., 1975; Page and El-Hosseiny 1976; Eder et al., 2008), tree species (Jayne, 1959, 1960), moisture content (Jentzen, 1964; Spielberg, 1966; van den Akker et al. 1966; Ehrnroot and Klosteth, 1984), fiber position within the tree (Burgert et al., 2005; Groom et al. 2002a and b) pulping process (Leopold, 1966,1968; Page, 1983, Burgert et al., 2005). Based on data from Page and El-Hosseiny (1983) it can be observed that single fiber tensile stress-strain curves have a gradual transition from elastic behavior to an elastic-plastic non-linear behavior, as shown in Figure 1. In different studies, bond strength between cellulose fibers has been found to be within the interval 0-10 MPa (Schniewind et al., 1964; Mohlin 1974).
Papers made from pulp fibers will be anisotropic, because fibers have a tendency of forming an anisotropic fiber structure during the papermaking process. In paper made on paper machines most fibers will be oriented in the plane of the paper; where most fibers will be in the machine direction (hereinafter referred to as MD), and fewer in the cross machine direction (hereinafter referred to as CD). The number of fibers oriented in the through-thickness direction (hereinafter referred to as ZD) will be few. Due to the fiber structure, the stiffness in the MD can be 1 to 5 times higher than in CD, moreover the MD stiffness can be a factor 100 stiffer than the ZD stiffness (Baum et al. 1981).

The purpose of this study is to propose a micromechanical network modeling strategy and a constitutive model for fibers, with material data fitted to the single fiber stress-strain curves from Page and El-Hosseiny (1983), in order to investigate the influence of fiber properties on paper properties. This modeling strategy is different from most other micromechanical models that has been used to study paper. The most common strategy in the literature has been to represent the fibers by bonded beam elements (Wang and Shaler, 1998; Heyden, 2000; Bronkhorst, 2003; Pawlak and Keller, 2005; Kotik, 2007; Hägglund and Isaksson, 2008; Kulachenko et al., 2009). Here instead, the ideas proposed by Niskanen et al. (1997) are developed, where a model paper is created by deposition of idealized fibers on a square lattice.
2. Model
A network model that represents paper will be proposed, where the particular aim was to represent the fibers and network structure adequately. The aim is to mimic the network structure of e.g. paperboard which can be seen in Figure 2.

![Cross-sectional view of a paperboard network structure.](image)

Figure 2: Cross-sectional view of a paperboard network structure.

To investigate the importance of fiber properties it is important to generate a representative volume element of the paper. Hence, several fibers need to be investigated, and different types of deformations of the fibers and network need to be investigated. Therefore, each fiber was treated as a continuum. In order to investigate the importance of fiber properties for paper materials, single fiber data was assigned to the fibers. This was done using an isotropic elastic-viscoplastic model that previously has been used to study polycarbonate (Anand and Gurtin, 2003).

2.1 Representative volume element (RVE)
The size of the RVE will be chosen such that it contains several fibers, and will capture the essence between different loading directions due to fiber orientation. As a consequence, the size of RVE was chosen to be $1.59 \times 1.59 \times 0.40 \text{ mm}^3$. The micromechanical modeling was done by using Abaqus/Explicit (Abaqus, 2009). A mesh consisting of $10 \times 10 \times 10$ eight-noded linear elements, C3D8 (Abaqus, 2009), was generated. The mesh was constrained by periodic boundary conditions, where constraints of all outer boundaries was formulated using the definition of strain:

$$u^A_t - u^B_t = \bar{e}_{ij}(x^A_j - x^B_j).$$  \hspace{1cm} (1)

The periodic boundary conditions were implemented using dummy nodes and constraint equations (Abaqus, 2009). More details about the periodic boundary condition and the representative volume element can be found in Nygård’s (2003), where a similar model has been used to study grain structures in metals.
2.2 Network model

In the model, a fiber with total length $L$ and with global orientation $\theta$, in the MD-CD plane measured from the MD direction, was generated. Moreover, the fiber was divided into a number of segments, in this study 10. Each segment was assigned an additional rotation $\theta_i$, measured from the primary rotation $\theta$. A kinked fiber could then be generated, as seen in Figure 3a. Since the fiber was larger than the RVE it was fitted into the RVE by making the fiber periodic within the RVE. This means that the fiber that was characteristic for a paper material, was utilized to generate a periodic network structure within the RVE. Hence, the fiber generated a network structure within the RVE, as seen in Figure 3b.

![Figure 3: a) A typical fiber and b) The same fiber that has been made periodic within the RVE.](image)

To mesh the fiber, i.e. to divide the RVE into fibers or voids, all element that had its middle point within the fiber diameter $d$ ($d = 0.027$ mm) were assumed to belong to the fiber, as illustrated in Figure 4. A consequence of this assumption was that the fiber form will depend on the element size. If a finer mesh is used, the fiber will be less kinked.
Figure 4: The randomly generated discretized fibers in the ten different layers of the RVE.
For each element layer in the thickness direction (i.e. totally 10 layers) one fiber that has been made periodic was generated. Hence, it was predefined that the fiber thickness was 0.04 mm. It also had the consequence that each fiber lies in the MD-CD plane. In Figure 4, the fibers have been plotted as thin line for clarity, while the elements represent the assigned fibers. The remaining elements, white in Figure 4, were assumed to belong to element set, void. The void elements were also present in the simulations, but their properties were more compliant in order not to interfere with the fibers. The three-dimensional mesh representing the fibers can be seen in Figure 5.

![Figure 5: The meshed RVE, which contained 10*10*10 elements and was loaded by periodic boundary conditions.](image)

The purpose of the generated RVE was to investigate fiber deformation mechanisms. Therefore, the fibers were meshed using continuum elements, since this enabled studies of elastic-plastic deformation, as well as bending of the fibers. In this study the bonds were assumed to be infinitely strong, i.e. debonding of fibers was not possible. This was a course approximation of paper behavior. However, this approximation made it possible to study the effect of fiber properties in the network.

2.3 Fiber model

In Figure 1, it can be observed that fibers with high fibril angle exhibit a plastic behavior that has an initial linear region followed by an additional hardening effect with an increased hardening modulus. For polycarbonate, a similar behavior has been observed, where the interpretation is that amorphous regions of the plastic become ordered since polymer chains straighten (Anand and Gurtin, 2003). A constitutive framework for this behavior has been proposed by Anand and Gurtin (2003), which has been implemented into Abaqus/Explicit as a VUMAT (Abaqus, 2009) by Bonnaud and Faleskog (2010). The model is shortly described below; it is based on hyperelasticity and on the multiplicative split of the deformation gradient \( F = F^e F^p \). The conjugate measures for
Plasticity features both isotropic and kinematic hardening. With \( \nu^n_P \) being the equivalent plastic shear strain rate, \( \eta \) a measure of the local free volume and \( \{ h_0, g_0, s_0, s_{cv}, b, \eta_0, \eta_{cv} \} \) material parameters, the isotropic hardening \( s \) is solution of the following equation system:

\[
\begin{aligned}
\dot{s} &= h_0 \left(1 - \frac{s}{\bar{s}}\right) \nu^p \\
\dot{\eta} &= g_0 \left(\frac{s}{s_{cv}} - 1\right) \nu^p
\end{aligned}
\]  

(4)

where \( \bar{s} = s_{cv}[1 + b(\eta_{cv} - \eta)] \) and \( s(0) = s_0 \) and \( \eta(0) = 0 \).

The kinematic hardening \( S^b \) is entirely derived from the left plastic Cauchy-Green deformation tensor \( B^p = F^p F^p T \). An effective plastic stretch \( \lambda^p \) is introduced and used to define the back stress modulus \( \mu \). The Langevin function is defined by \( L(x) = \coth(x) - 1/x \) for \( x > 0 \) and its inverse is denoted \( L^{-1} \); \( \{ \mu_R, \lambda_L \} \) are material parameters. Accordingly:

\[
\begin{aligned}
\lambda^p &= \sqrt{\text{tr}(B^p)/3} \\
\mu &= \mu_R \left(\frac{\lambda_L}{3\lambda^p}\right) L^{-1}\left(\frac{\lambda^p}{\lambda_L}\right)
\end{aligned}
\]  

(5a, 5b)

Taking the deviatoric part of \( B^p \) and multiplying it by \( \mu \) gives the back stress tensor \( S^b \):

\[
\begin{aligned}
B^p_0 &= B^p - \frac{1}{3} \text{tr}(B^p) I, \\
S^b &= \mu B^p_0
\end{aligned}
\]  

(5c, 5d)

The creep law is hydrostatic pressure dependent while the plastic strain directions are orthogonal to the load function (corresponding to the yield surface for inviscid plasticity). In that sense the model can be said to feature non-associative plasticity.
The equivalent shear stress $\bar{\tau}$ is defined from the deviatoric Cauchy stress $T^e_0$ and the back stress tensor $S^b$:

$$\bar{\tau} = \frac{1}{\sqrt{2}} |T^e_0 - S^b|.$$  \hfill (6a)

With $\{v_0, \alpha, m\}$ being material parameters, expressions for the equivalent plastic shear strain rate $\dot{\gamma}^P$ and the plastic strain rate tensor $D^P$ read:

$$\dot{\gamma}^P = v_0 \left( \frac{\bar{\tau}}{\tau + \alpha \pi} \right)^{\frac{1}{m}},$$  \hfill (6b)

$$D^P = \nu^P \left( \frac{T^e_0 - S^b}{2\bar{\tau}} \right).$$  \hfill (6c)

### 2.4 Determination of material constants

The material constants that affected the elastic-plastic behavior of single fibers were determined by approximately fitting the stress-strain curves to the single fiber data published by Page and El-Hosseiny (1983). The fitting was not made exactly, rather the purpose was to generate stress-strain curves that were resembling the published data, since the purpose of this study was to investigate mechanisms. For single fiber data, it was observed that as the fibril angle changes, the elastic-plastic behavior was altered. The key features were the elastic modulus, the yield stress and the initial hardening. All these could be well represented by a linear interpolation depending on the fibril angle, as seen in Figure 6.

With the proposed constitutive model the elastic-plastic behavior was determined as function of the fibril angle. To fit the single fiber data five material parameters were expressed in terms of fibril angle, $\phi$, hence:

$$K = 18000 + 55000 \frac{46 - \phi}{46} \text{ MPa},$$

$$G = 8000 + 18000 \frac{46 - \phi}{46} \text{ MPa},$$

$$\mu_R = 40 \frac{46 - \phi}{46} \text{ MPa},$$

$$\lambda_L = 1.05 + 0.003 \frac{\phi - 4}{36},$$

$$s_0 = 200 + 700 \frac{46 - \phi}{46} \text{ MPa},$$

where $\phi$ was expressed in degrees in the interval $1^\circ < \phi < 46^\circ$. The remaining parameters were assumed to be constant and set to: $v_0 = 0.0017 \text{ s}^{-1}$, $m = 0.011$, $\alpha = 0.08$, $h_0 = 160 \text{ MPa}$, $b = 200$, $s_{cv} = 20 \text{ MPa}$, $g_0 = 0.00006$ and $\eta_{cv} = 0.001$.

The resulting stress-strain curves for single fibers with different fibril angles, represented by the material data above are shown in Figure 7.
Figure 6: a) Evaluated data of elastic modulus $E$, hardening modulus $H$ and b) Initial yield stress, $\sigma_s$, from single fiber measurements published by Page and El-Hosseiny (1983).

Figure 7: Stress-strain curves with the proposed constitutive model and the material data used in the simulations.
The void elements were assumed to be isotropic and elastic with elastic modulus $E = 2000 \text{ MPa}$ and Poisson's ratio $\nu = 0.3$.

3. Results and discussion
Random fibers with length uniformly distributed in the interval $3.5 \text{ mm} < L < 4.5 \text{ mm}$ and width $0.027 \text{ mm}$ with global directions uniformly distributed in the interval $-\pi/16 < \theta < \pi/16$ and local segment direction uniformly distributed in the interval $-\pi/8 < \theta_i < \pi/8$ were generated. This model generated a network where the fiber coverage was 27.1%, i.e. 271 elements were fibers and 729 elements were voids. All 10 layers of fibers can be seen in Figure 4.

3.1 Simulation of uniaxial tensile tests in MD, CD and ZD
The micromechanical model was used to study uniaxial tensile tests in MD, CD and ZD, as seen in Figure 8. Loading by an average strain $\bar{e}_{ii} = 0.1$, where $ii = xx, yy$ and $zz$, was performed for models that consisted of fibers with fibril angles $\phi = 4^\circ$ and $\phi = 40^\circ$. These fibril angles were chosen since they represent the extreme cases of fiber properties; $\phi = 4^\circ$ was almost linear elastic, while $\phi = 40^\circ$ was elastic-plastic with an increased hardening effect when $\bar{e}_{xx} = 0.05$, as seen in Figure 8.

![Simulated stress-strain curves in MD, CD and ZD for networks containing 27.1% fibers coverage with fibril angles $\phi = 4^\circ$ and $\phi = 40^\circ$.](image-url)
It should be kept in mind that the micromechanical model does not include a failure criteria, therefore it can be loaded further than the corresponding experiments. Although, the fibers are represented by an isotropic model, the loading in MD, CD and ZD have different stiffness, as seen in Figure 8, which is due to the generated fiber orientations. Hence, different fiber deformation mechanisms were activated. For loading in CD and ZD more fiber bending, in relation to fiber stretching, was activated than in MD. Hence, papermakers that can constrain flexibility within the network structure should also be able to utilize the fiber stiffness better.

In the micromechanical model, tension in the fiber was assumed to be the dominating deformation mechanisms, since uniaxial tensile data was used as input to the fiber data. The resulting elastic moduli for the network and its relation to the respective fiber modulus, $E_{fib}^4$ and $E_{fib}^{40}$, then took the values given in Eq. 8. For loading in MD with stiff fibers it was observed that the model followed the rule of mixture quite well, since $\frac{E_{MD}^4}{E_{fib}^4}$ and $\frac{E_{MD}^{40}}{E_{fib}^{40}}$ were close to the volume fraction of fibers.

\[
\begin{align*}
E_{MD}^4 &= 16733 \text{ MPa} \quad \frac{E_{MD}^4}{E_{fib}^4} = 0.26, \\
E_{MD}^{40} &= 8009 \text{ MPa} \quad \frac{E_{MD}^{40}}{E_{fib}^{40}} = 0.30, \\
E_{CD}^4 &= 9867 \text{ MPa} \quad \frac{E_{CD}^4}{E_{fib}^4} = 0.15, \\
E_{CD}^{40} &= 6165 \text{ MPa} \quad \frac{E_{CD}^{40}}{E_{fib}^{40}} = 0.23, \\
E_{ZD}^4 &= 4798 \text{ MPa} \quad \frac{E_{ZD}^4}{E_{fib}^4} = 0.08, \\
E_{ZD}^{40} &= 4101 \text{ MPa} \quad \frac{E_{ZD}^{40}}{E_{fib}^{40}} = 0.15.
\end{align*}
\]

However, it was somewhat lower for loading in CD and ZD, mainly since fiber bending could be activated to a larger extent in these simulations. The in-plane elastic modulus for the network with $\phi = 40^\circ$ was similar to what has been experimentally observed for the different plies in paperboard (Nygård, 2008), while the in-plane elastic modulus for the fibers with $\phi = 4^\circ$ was somewhat higher. Moreover, the absolute stress levels for ZD loading were higher than for paper materials. In the model all elements were assumed to be perfectly bonded, hence loading conditions where debonding is an important deformation mechanism stress will become too high.

In the model, plastic deformation was activated already when $E_{MD} = 2\%$ for MD, which is close to the fiber yield point for fibers with $\phi = 40^\circ$, hence there is a uniform strain field for MD loading, as supported by the contour plot in Figure 9a and b.

In CD, the strain field was not as uniform, see Figure 9c and d, and hence the stress-strain curve had
a smoother shape into the plastic regime, and the yield point came roughly when $\varepsilon_{cd} = 2\%$. For ZD loading, the straining of the fibers was much less pronounced, since fiber bending was to a larger extent enabled. Therefore the local strain in the elements was low, as observed in Figure 9e and f. For ZD loading the resulting stress-strain curves were mainly elastic, and the dominating damage mechanism, in a real paper, would be bond failure. Since this was not accounted for here, the stress level in the resulting stress-strain curve became too high, both with respect to stiffness and strength. Normally the stress levels between MD and ZD differ a factor 100 (Nygård, 2008).

Figure 9: Iso-contours of principal logarithmic strain at average strain level of 0.01 for uniaxial loading in a) MD with $\phi = 4^\circ$, b) MD with $\phi = 40^\circ$, c) CD with $\phi = 4^\circ$, d) CD with $\phi = 40^\circ$, e) ZD with $\phi = 4^\circ$, f) ZD with $\phi = 40^\circ$. 

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In the simulations there is large difference between the networks with $\phi = 4^\circ$ and $\phi = 40^\circ$. In the latter, the plastic behavior is dominating, while the former is mainly elastic. In a network, the fibers have random fibril angles. Fibers with high fibril angle would then deform plastically when loaded in tension and give rise to a non-linear response. The mechanisms behind the additional hardening effect would be tightening of the fibrils. It is however reasonable to assume that also fibers with low fibril angle would show this non-linear behavior when loaded in torsion. However, experimental support for this hypotheses is lacking. If this were the case, one would be able to observe an additional hardening effect in papers after approximately $\varepsilon = 5\%$, which would indicate that the properties of the fibers are utilized more efficiently. This additional hardening effect can be observed in commercial paper grades, as exemplified by a paperboard sample in Figure 10.

In the literature also sack paper has been observed to have this additional hardening. The non-linearity in the stress-strain curve would indicate that the fiber properties are well utilized.

Figure 10: Example of a paperboard loaded in CD tension, where an addition hardening effect is seen for large strains.

4. Conclusions

A micromechanical modeling concept was proposed to investigate the effect of fiber properties on the paper network properties. By using continuum elements and an isotropic material model anisotropic network properties could be simulated by using an anisotropic fiber orientation. Anisotropic paper properties could be predicted for uniaxial tension tests in MD, CD and ZD. The material model, that was utilized to represent fiber properties, had an additional hardening effect at large strains that has been observed experimentally for single fibers with high fibril angle. In was observed that this fiber behavior also could be observed for paper network properties. Hence, papers that show this hardening behavior, such as sack paper, utilizes the single fiber properties well.
Acknowledgment
The financial support from BiMaC Innovation is gratefully acknowledged.

References


