Modeling the in-plane mechanical behavior of paper

A literature survey

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Abstract

Paper and paperboard are widely used in packaging for transportation, storage and retail. Increasing demands on the shapes and mechanical durability of these products require innovation of their manufacturing techniques. Conventional trial-and-error paper product development processes prevent rapid and cost-efficient adaptations in production. Mechanical models, that can predict the mechanical properties of paper efficiently and effectively, have the potential to overcome this issue. It appears that in this respect, models that are currently available leave room for improvement. Therefore, this report lays a foundation for the further development of such a model. First, the geometric and mechanical properties of the fibrous network of which paper consists are analyzed. An inventory of the models that have been used to model paper’s in-plane mechanical behavior is given, in which a distinction is made between continuum models and discrete models. The former appear to be quite accurate but complex; the latter are simpler but leave room for improvement. Therefore, considerations in composing a special type of discrete models, called lattice models, are elaborated. Emphasis is put on modeling the behavior of individual fibers and fiber bonds, and how these models may be formulated to accurately simulate the in-plane mechanical behavior to failure of paper.
Chapter 1

Introduction

Paper and paperboard are widely used in packaging for transportation, storage and retail. The processing of paper materials into packages requires a series of manufacturing steps, many of which involve rapid plastic deformation of the paper(board) in mass production.

Manufacturers encounter various difficulties in making paperboard products profitable in the future, by delivering high-quality products in large volumes at low cost. For instance, paperboard typically loses much of its favorable mechanical properties if exposed to environments with a low or high relative humidity, as during winter time. In retail, increasing demands on the appeal of a cardboard package require technically more complicated package shapes. Overcoming such issues and making paperboard products meet the quality that tomorrow’s markets demand could be highly lucrative for manufacturers. This is a strong incentive to examine the possibilities of improving their products. However, conventional trial-and-error paperboard product development stands in the way of rapid and cost-efficient improvements.

A measure to streamline this process is to use a numerical model, that can easily and adequately simulate the mechanical behavior of paper and paperboard. The use of such a model would make tedious and costly testing procedures redundant. To the best of the author’s knowledge, no model exists at the moment that has the capacity to predict the mechanical behavior of paper when subjected to destructive deformation both efficiently and effectively. This literature survey serves as a basis for the development of a model for this purpose.

To get a clear image of what is to be modeled in the first place, a characterization of paper is given in chapter 2. The microstructure of a network of fibers that are connected by bonds is described, as well as how the effective mechanical behavior is influenced by various aspects of this structure.

Chapter 3 highlights some of the progress in paper modeling that has been found in the literature. A distinction is made between models that rely on a continuum approach and discrete models (particularly lattice models). It appears that the continuum modeling of paper has yielded realistic results but is quite complex. On the other hand, the few lattice models of paper that exist are relatively straightforward, but their ability to accurately simulate paper’s mechanical behavior from small deformations to complete failure is yet to be comprehensively demonstrated.

Since lattice models appear to allow for a more natural incorporation of damage (progression) that continuum models, chapter 4 lays a foundation for the creation of an accurate lattice model for paper by discussing considerations in the composition of such a model. Emphasis is put on fiber and bond failure mechanisms, which seem to play an important role in the incorporation of the onset and progression damage in a lattice. The successful modeling of these phenomena in a lattice for paper has not been encountered in the literature up to this day.
Chapter 5 comprises a concluding discussion of the potential pitfalls and opportunities in the construction of a lattice model to describe the mechanical behavior of paper and paperboard.
Chapter 2

Paper characteristics

2.1 Production process

To produce paper, harvested wood is defibered and the separated wood fibers are diluted into a low-content suspension, referred to as pulp [1, 2]. A turbulent flow of the pulp is filtered by a wire mesh, resulting in fiber sedimentation and aggregation on the wire. After drainage, the planar network of fibers is pressed between felts to increase its density, and more water may be evaporated. The fibers in the network have an orientational preference in the ‘machine direction’ (MD) due to the difference in speed between the suspension flow and the wire. The perpendicular in-plane direction is called ‘cross direction’ (CD) and the out-of-plane direction is referred to as ‘thickness direction’ (TD or ZD). A simple illustration of these directions in a paper sheet is given in figure 2.1.

![Figure 2.1: Illustration of the principal directions of paper’s structure: machine direction (MD), cross direction (CD) and thickness direction (TD or ZD). The sheet represents the planar fibrous microstructure.](image)

2.2 Paper topology

Due to the wet fiber deposition process and pressing as described above, paper is a planar material that consists of layers of densely packed cellulose fibers, that is conventionally considered to be linked by primarily hydrogen bonds [3]. An image of the fibrous structure of paper on a microscopic level is given in figure 2.2.

The density of such networks varies per paper type, and is often expressed as the mean fiber length and number of fiber interactions per unit area. Such parameters have been quantified by various studies, both numerically [1,4–6] and experimentally [7]; the latter is limited by the poor contrast obtained. These density-dependent properties have a profound impact on paper’s mechanical properties [3,8], as subsequent sections will further illustrate.
The in-plane orientation of the fibers is often described by a Gaussian distribution with its mean in machine direction [3], as is illustrated in figure 2.3.

An implication of the fiber damage involved with wood defibration and the turbulent wet fiber deposition on the wire, is that fibers are generally curled and kinked when consolidated in the sheet [1,9], as figure 2.2 shows.

2.3 Mechanical properties of paper components

2.3.1 Individual fibers

Much is known about the geometric and mechanical characteristics of individual fibers [3,9], and especially how these characteristics depend on the type of wood and the production process to turn them into paper. A detailed examination of these relations lies beyond the scope of the present research, which focusses on modeling effective phenomenological characteristics of paper
(and similar fibrous materials). Therefore, only directly relevant mechanical properties are considered here on a qualitative level.

In a literature review by Niskanen [3], it is noted that fibers without defects are linear elastic or nearly so. Curls and defects (e.g., crimps, kinks, micro-compressions rectified by elongation) that are present in paper's fibrous microstructure often lead to considerable non-linearity in the fiber mechanical behavior. As the fiber stress-strain curves of figure 2.4 show, the ratio between the initial (near-)elastic regime and the amount of plasticity that a fiber shows is strongly determined by a certain material orientation in a layer inside the fiber, called the fibril orientation. Variations in such detailed structural features are some of the reasons that accurate and useful determination of fiber mechanical properties is complex. Different stress-strain curves found in the literature indicate that the fibers are generally linear elastic followed by elastic-plastic behavior until failure, with a typically smooth transition between the two regimes.

Figure 2.4: Stress-strain curves that illustrate the qualitative mechanical behavior of fibers for different fibril angles of black spruce fibers [10].

2.3.2 Inter-fiber interactions

The characteristics of inter-fiber interactions have been examined in the literature. The following is based on a book by Niskanen [3], unless indicated otherwise.

An inter-fiber bond is defined as the zone where two fibers are close enough to each other to have significant interaction. The exact geometry of bonds is hard to characterize, due to the stochastic structure of fiber surfaces and the delicacy of the organic material of the fibrous structure. Some experimentally found values of bond area are in the order of $10^3 \mu m^2$.

Based on the type of interaction, three types of bonding can be defined: chemical bonding, intermolecular Van der Waals bonding and entangling. The inter-fiber bonds in paper are probably a combination of these types, where it may be difficult to make a clear distinction. Hydrogen bonds, a special type of chemical bonds, is conventionally considered to be an important element of the inter-fiber bonds in paper.

In characterizing the mechanical behavior of bonds, it is difficult to make a clear-cut definition and measurement of the complex and delicate inter-fiber connections: e.g., bonds may
fail non-uniformly due to a non-uniform stress distribution (see figure 2.5). Not surprisingly, a comprehensive characterization of the constitutive behavior of bonds has not been found in the literature. Some mechanical properties, however, have been described, which are briefly discussed in the following.

Shear strengths of bonds in a certain paper type (made from Loblolly pine) are reported to be in the range $5 \text{mN} - 11 \text{mN}$; it is unclear which experimental techniques were used to obtain these values. In one experiment \[11\], estimations of bond strengths are made from the pullout of individual fibers from a well-bonded paper sheet. The results suggest that bond strengths in the used paper type are approximately $5 \text{mN} - 8 \text{mN}$.

Note that, using the above data, the maximum shear stress of a bond cannot unequivocally be taken as the estimated bond strength divided by the bond area. The measured bond area is not necessarily the bond area at the moment of failure, and the non-uniform stress distribution in bonds makes such conclusions even more questionable.

Andersson and Rasmuson \[12\] have managed to quantify the friction characteristics between pulp fibers that slide along each other. Measurement results for the coefficients of friction for dry and wet pulp fibers are listed in table 2.1.

![Figure 2.5: Schematic of stresses in the bonds. Left: tension-free situation, residual bond stresses from production process. Right: bond stresses when subjected to tension \[23\].](image)

<table>
<thead>
<tr>
<th>dry pulp</th>
<th>$\mu$</th>
<th>$\bar{s}$</th>
<th>$s_f$</th>
<th>$n_m$</th>
<th>$n_f$</th>
<th>wet pulp</th>
<th>$\mu$</th>
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<td>0.20</td>
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<td>15</td>
<td>Kraft</td>
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<td>0.10</td>
<td>0.16</td>
<td>61</td>
<td>8</td>
</tr>
<tr>
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<td>0.18</td>
<td>0.21</td>
<td>79</td>
<td>14</td>
<td>TMP 514</td>
<td>0.92</td>
<td>0.13</td>
<td>0.15</td>
<td>46</td>
<td>8</td>
</tr>
<tr>
<td>TMP 700</td>
<td>0.80</td>
<td>0.17</td>
<td>0.30</td>
<td>61</td>
<td>6</td>
<td>TMP 700</td>
<td>0.97</td>
<td>0.18</td>
<td>0.24</td>
<td>35</td>
<td>7</td>
</tr>
</tbody>
</table>

**Table 2.1:** Measured values for the average coefficient of friction between two fibers $\mu$, the mean standard deviation of single fiber measurements $\bar{s}$, the standard deviation for average measurements between fibers $s_f$, number of measurements $n_m$ and number of tested fibers $n_f$ \[12\].

### 2.4 Effective in-plane mechanical behavior of paper

The microscopic characteristics of paper are reflected in its macroscopic mechanical behavior. As a result of the fibers’ orientational preference, paper is anisotropic. The three principal directions (i.e., MD, CD, TD) are the symmetry axes for the mechanical behavior; hence, paper is regarded
as an orthotropic material [1]. The orthotropic properties of paper are described in more detail in the subsequent sections.

2.4 Elastic properties

As is described in the book by Niskanen [3], most paper types show linear elastic behavior during initial straining. The relations between the fibrous microstructure and effective elastic properties are much better understood than the micro-macro relations of other mechanical properties (e.g., that describe failure), due to their statistical stability. Various studies have experimentally determined paper’s elastic properties (e.g., Gooren [13]) and also analytical-numerical models have been used to model elastic properties: e.g., Schulgasser [14], Ostoj-Starzewski and Stahl [15].

A widely discussed elastic property is the Young’s modulus, or more specifically for paper, the Young’s moduli in the three principal directions. As Niskanen [3] has described, the in-plane Young’s moduli (i.e., the moduli in MD and CD) are measured in tension, while the out-of-plane modulus (in TD) is generally determined in compression. The tensile and compressive moduli may differ as a result of fiber bending and buckling. Reported values of elastic moduli, for various types of paper after different production processes, are approximately in the range of \(E_{MD} = 0.2\text{GPa} - 9\text{GPa}\). The considerable diversity in these numbers indicates how dependent the moduli of paper are on various parameters, such as morphological characteristics due to differences in production. Page and Seth [16] have experimentally identified that some of the most important features in this respect are inter-fiber load transfer limitations and fiber defects: i.e., microcompressions, curls and kinks. A key parameter in the modulus of paper is the fiber network density, as is reflected by the fact that most (production process) influences on paper’s elastic modulus are visualized in terms of the elastic modulus as a function of density. Typically, these graphs are linearly increasing.

The Poisson ratio is another elastic property, which is described by Niskanen [3]. In isotropic paper such as handsheets, its in-plane value is \(\nu \approx 0.3\). More generally, values have been reported in the range \(0.1 < \nu < 0.5\). In thickness direction, the Poisson ratios vary considerably, and they can even be negative.

The shear modulus is an important elastic parameter for packaging boards [3,17]. Niskanen [3] has explained that in paper webs, shear stresses arise if the main fiber orientation angle is not in MD. This causes web wrinkling, which impedes the accurate measurement of the shear modulus. Shear moduli are therefore often estimated from elastic moduli in MD and CD [3,14]; a rule of thumb is \(G \approx 1/3\sqrt{E_{MD}E_{CD}}\). Alternatively, the in-plane shear modulus can also be derived from tensile tests that are performed under a 45° angle with MD and CD, using elasticity theory and the assumption of plane stress [13].

2.4.2 Onset of plasticity

Niskanen [3] has described that paper is not purely elastic; the typical stress-strain behavior until failure is qualitatively illustrated in figure 2.6 for both in-plane principal directions. After initial elasticity, paper yields (typically after some tens of percents strain) and subsequently shows elastic-plastic deformation until the onset and progression of damage [3,9]. Note that some stress-strain curves found in the literature may show a small initial ‘run-up’ to linear elasticity [13]; this is the result of only partial load-carrying of the fibrous network, which can be avoided by pre-straining a sample.

The constitutive behavior of paper is highly similar to the constitutive behavior of fibers, as described in section 2.3.1. This is no coincidence; as Niskanen [3] has described, a primary deformation mechanism in the elastic-plastic regime is the elongation of the elastic-plastic fibers.
In the elastic-plastic deformation regime, this microscopic phenomenon is accompanied by the gradual opening of the inter-fiber bonds. The bonding degree is reported to have no qualitative effects on the stress-strain behavior of paper up to this level of strain. How bond failure can play a significant role in this respect is described in section 2.4.3.

As illustrated in figure 2.6, Niskanen [3] has argued that the stress-strain slope under plastic deformation (before damage significantly affects the response) is higher in MD than in CD. This causes paper to reach its strength (i.e., maximum stress before failure) at a considerably lower strain level in MD (∼1.8% strain) than in CD (∼3.3% strain). The Young’s modulus for MD ($E_1$ in figure 2.6) is clearly higher than the modulus in CD ($E_2$).

How the modulus is affected during elastic-plastic deformation can be visualized by a stress-strain curve of cyclic loading, such as figure 2.7 by Gooren [13]. This curve indicates that the Young’s moduli of initial loading and reloading are virtually identical, so for each in-plane direction, the Young’s modulus seems hardly affected by straining. Specifications of this relation for
the entire straining domain by Niskanen [3] (see figure 2.8) indicate that the reloading modulus is only limitedly affected by strain; in MD it seems to decrease approximately by 10% over the entire straining domain and in CD no distinct relation can be identified due to scatter in the measurement results. When assuming that the modulus is not distinctly affected by straining, the (recoverable) elastic strain at any point in the loading curve can be determined (by approximation) as $\epsilon_{el} = \sigma/E$.

![Figure 2.8: Measurement results of the Young's modulus as a function of stress in machine direction (top) and cross direction (bottom) [3].](image)

It should be noted that the mechanical behavior of paper is deformation rate sensitive [3, 9]. Stresses are significantly amplified over the entire straining domain when a higher strain rate is used, as figure 2.9 shows. Increasing the strain rate can significantly lower the tensile strain and increase tensile stress. Paper is therefore characterized as a visco-elastic plastic material.

### 2.4.3 Failure

As Isaksson et al. [18] have described, damage occurs from a particular macroscopic strain $\epsilon_D$ in the elastic-plastic domain. This is reflected in the stress-strain curve shown in figure 2.10, as for $\epsilon > \epsilon_D$ (indicated in the left figure) stresses start to drop under progressive straining and deviate from the fictive damage-free stress-strain characteristic (blue curve in the right figure). Initially, this damage is distributed over the paper specimen and stresses drop as damage increases in the network. At a certain strain level, localization occurs and damage becomes locally progressive: i.e., the specimen starts to fracture. This is reflected in the clear drop in stress in the stress-strain curve of figure 2.10, which can only be measured if the damage process is stable. Note that for packaging materials, this behavior can only be obtained at a relatively short gauge length [29]. The subsequent tail of the stress-strain curve indicates that some fibers still carry load. As soon as the fracture has grown into a complete separation zone of two parts of the fibrous network, the sample loses all of its load-carrying capacity.

Examination of fractured specimens revealed that bond failure is the distinctly dominant mechanism compared to fiber failure. It has been observed [3, 19] that complete bond failure is rare; most bonds have opened gradually and did not break completely even when paper is strained to
2.4 Effective in-plane mechanical behavior of paper

Figure 2.9: Illustration of the sensitivity of the mechanical response of (MG) paper to the strain rate [3].

failure.

Figure 2.10: Typical stress response of a paper specimen to uniaxial tensile straining. The black lines connect measured values. In the left figure the strain that corresponds of damage onset $\epsilon_D$ is indicated. In the right figure, the blue line indicates the theoretical stress-strain behavior if no damage would have occurred; how the blue curve relates to the black curve is an indication for the amount of damage $D$ [18].

Note that the curling of fibers appears to have an influence on the failure of paper, as Perez and Kallmes [20] have identified. A larger distribution in fiber curl is concluded to have a negative influence on the strength of paper, since more fibers have to be stretched and thereby do not fully contribute to the load-carrying capacity of the paper. This stretching does increase the extensibility of paper before total failure. It is conceivable that both highly extensible and strong paper can be made by utilizing highly curled fibers with a uniform curl.
Chapter 3

Modeling of paper’s in-plane mechanical behavior

Paper’s mechanical behavior has been modeled in various ways in the past, as will become clear in this chapter.

Section 3.1 gives an overview of some of the most remarkable achievements in the modeling of paper’s mechanical behavior using a continuum approach. Section 3.2 summarizes noteworthy results in the field of discrete modeling of paper, wherein emphasis is put on a type of discrete models called lattice models. A concluding discussion of these models is given in section 3.3, where their capabilities in conveniently modeling the mechanical in-plane behavior of paper to failure are compared.

3.1 Continuum models

This section, on the results of continuum models for paper, is subdivided in three parts. First, the modeling of paper’s elastic behavior is given in section 3.1.1. Section 3.1.2 mentions results of studies that have incorporated elastic-plastic behavior in their model. Finally, the modeling of damage in paper using a continuum approach are discussed in section 3.1.3.

3.1.1 Elasticity

In the second half of the 20th century, much work has been done spanning the size range between fiber and sheet for the elastic properties of paper by the use of a continuum approach [1, 9]. Most of these studies have modeled fibrous materials as composites that are assumed to behave elastically under uniaxial tensile straining. A classic in this field is a paper by Cox [21], who has regarded a sample of long oriented fibers embedded in a matrix. This paper derived an expression for the effective modulus of this fibrous structure using shear-lag theory. Campbell [22] has derived a more specific long fiber model and obtained the same result. Van den Akker [23] has constructed a model that no longer assumes that the fibers are embedded in a matrix. This model includes rigid bonds between fibers and allows for fiber bending and shear in addition to axial strain. A distinction in bond failure has been made between shear stress resulting from tension in the fibers and torque due to fiber rotation. Perkins and Mark [24] have presented a continuum model that incorporates an independent deformation variable that describes the rotation of fiber segment ends which are bonded together. To approximately simulate the effects of bond flexibility (extension, shear, bending), the authors have taken the fiber length to be the distance between two bond centroids. Page and Seth [16] have noticed that the presence of inter-fiber load transfer limitations and fiber defects (i.e., microcompressions, curls, kinks) in paper limits the ability of
3.1 Continuum models

the Cox model to accurately predict the modulus. The authors have therefore constructed a model that enables the prediction of the global modulus if these morphological features are significantly present. A later paper by Qi [25] has regarded the expansion of a Cox-like model with a parameter that captures the degree of out-of-plane fiber orientation, as an early step towards 3d modeling. For more information, Heyden [1] has given an extensive overview of this field, which includes a summary of the expressions for the effective elastic modulus that have been derived by the models cited above.

3.1.2 Elastic-plastic behavior

Various publications have modeled the in-plane elastic-plastic behavior of paper, until damage occurs, using a continuum approach. Some works with noticeable findings will be discussed here.

Ramasubramanian and Perkins [26] have extended the elastic analysis of paper from previous works with the elastic-plastic behavior of fibers and bonds separately, as shown by the stress-strain curves in figure 3.1. These elements have been incorporated in a representative volume element, which is subjected to a deformation field. The results have been shown to be in quite good agreement with experimentally determined stress-strain data. For future work, the authors have recommended the modeling of in-plane fiber curl and extensive experimental testing.

Figure 3.1: Elastic-plastic constitutive behavior for the fibers (left) and the bonds (right) [26].

Xia et al. [27] have presented a phenomenological representation of paper in the form of a three-dimensional anisotropic continuum model under finite deformations. It comprises a multisurface yield function, anisotropic hardening and different behavior in tension and compression. The model is fitted to experimentally obtained stress-strain data of a certain type of paperboard. The fitted results have been shown to be in good agreement with the experimental data for both tension and compression, as figure 3.2 indicates for multi-axial tension.

3.1.3 Damage and fracture

The onset and progression of damage in paper has received considerable attention in the past decades [28]. In this context, some interesting studies that have treated paper as a continuum can be found in the literature. The results of some of these works are highlighted here.

Isaksson et al. [29] have modeled the in-plane mechanical behavior using a two-dimensional continuum model. This model includes gradient-enhanced continuum damage coupled to anisotropic plasticity. Rather than modeling two separate damage processes as in the real material (i.e., in the fibers and in the bonds), one damage mechanism has been modeled in which nothing is assumed on its nature. Isotropic damage hardening has also been included, to capture fracture in the model. Using experimentally obtained data from tensile experiments on two types of paper, the constitutive model has been calibrated and material parameters have been determined. The
stress-strain curves along MD and CD, that have been obtained by non-linear finite element analysis, fit the experimental data in the elastic regime well. The descending parts of the stress-strain curves have been reasonably well simulated after the numerical fitting of a hardening parameter and the application of an exponential damage evolution law; see figure 3.3.

If localization occurs, the failure process changes from a two-dimensional randomly distributed process to a one-dimensional process; the studying of this fracture process involves the application of different analytical techniques [28]. Despite that this reaches outside the realm of continuum mechanics, it is briefly treated here because the results are believed to be insightful. An example of a study that focused on the fracture process in paper is the publication by Niskanen et al. [30]. Based on the Griffith fracture energy analysis, the authors have derived how the fracture toughness of fibers depends on several other micromechanical parameters. They explained that the fracture toughness per fiber increases linearly with fiber length. Furthermore, as figure 3.4 shows, they...
demonstrated that there is an optimum in fracture toughness as a function of both bonding energy and fiber rupture energy: i.e., the energies required to break a bond or fiber respectively. The left graph shows that for a fixed fiber rupture energy, the fracture toughness can be optimized by tuning the bonding energy to a certain fixed value. The right graph illustrates the fracture toughness maximum as function of fiber rupture energy, for a fixed bond rupture energy. This suggests that the fracture toughness can be maximized by tuning the bond and fiber rupture energies relative to one another. Another work that has modeled the fracture process in paper is by Isaksson and Hägglund [28].

3.2 Discrete models

One way of analyzing the macroscopic mechanical properties of a fibrous material - paper in this case - is by composing a discrete model. A clear type of discrete models are lattice models. A lattice model consists of springs, trusses or beams that are connected to each other by nodes. An illustrative example of how a material (in this case, a specimen for tensile testing) can be represented by a lattice is shown in figure 3.5.

Lattice models have originally been designed to model materials on the atomic scale [31]. Since they may also be relevant at length scales much larger than that of molecular dynamics [32], they can be used to model material behavior on the macroscopic scale [31]. The discretized system of elements and nodes allows for a straightforward implementation of a material microstructure and included heterogeneities on a mesoscale [33]. If the (phenomenological) material constants (e.g., elastic moduli, yield thresholds) are properly set, the equations of motion of these lattices describe real materials even quantitatively [32].

Lattice models have been applied to a range of materials: e.g., textiles [34,35], metals [36] or composites [37]. However, to the best of the author’s knowledge, few lattice models have been
3.2 Discrete models

constructed to model paper so far. Studies to this end that have been found in the literature, are discussed in section 3.2.1. Section 3.2.2 highlights some findings of works that regarded materials with a quite similar microstructure or that do not apply to a specific material, which might be relevant in the present scope.

3.2.1 Application to paper

One of the clearest examples of lattice models for paper is the work by Bronkhorst [9]. Just like Xia et al. [27], Bronkhorst [9] has used experimental results to perform and validate numerical simulations of the elastic-plastic deformation of paper. Rather than using a continuum approach, however, Bronkhorst has composed a two-dimensional stochastic network model of elastic-plastic elements that are rigidly connected. This network, that mimics the microstructure of paper, has been subjected to in-plane stretching by simulation using a finite element code. As figure 3.7 shows, the numerically predicted and experimentally obtained curves of the in-plane mechanical response are in reasonable agreement. For further improvement, the author has recommended three-dimensional modeling (to decouple network grammage from network density) and the incorporation of a bond model which is more realistic than the rigid bonds that are used.

Figure 3.5: A lattice is used to model a material that undergoes deformation [42].

Figure 3.6: A (two-dimensional) RVE with a stochastic topology of rigidly bonded straight fibers [9].
3.2 Discrete models

In an attempt to also capture the failure process, Liu et al. [38] have recently proposed a two-dimensional lattice model for paper that incorporates bond failure. To simulate this failure, a threshold has been prescribed for the shear stress of the rigid bonds; if the shear stress reaches this value, the bond fails in a brittle manner: i.e., the two fibers that it connected are completely separated. Moreover, the elastic elements (that represent fibers) have been allowed to fail in a similar manner. Unfortunately, only qualitative results are given, and no comprehensive comparison of the results with experimentally obtained behavior of paper is made.

3.2.2 Other relevant applications

Some authors have constructed a lattice model for a material with a stochastic fibrous microstructure that is quite similar to that of paper.

A remarkable example is the work by Ridruejo et al. [39], who have modeled a glass-fiber non-woven felt by constructing a beam lattice unit cell with a topology that is similar to the one used by Bronkhorst [9]. They have been the first to propose a sophisticated bond model that includes the effects of energy dissipation by frictional sliding, which is inevitably involved with fiber pullout during failure. The results of this model, that are obtained using a finite element code, have proved to be in fair agreement with averaged experimentally found mechanical behavior, as figure 3.8 illustrates. The authors have also investigated the influence of choosing a different type of bonding, such as the rigid-brittle bond model like the one that has been used by Liu et al. [38]. Suggestions that are given for improving the accuracy of a model in predicting the in-plane mechanical behavior to failure of a non-woven felt include variations in network geometry and bond strength.

In her Ph.D. thesis, Heyden [1] has considered two- and three-dimensional lattice models of dry-shaped cellulose fiber fluff (e.g., material for diapers). She applied another sophisticated bond model to describe mechanical behavior to failure, which allows for capturing anisotropy, ductility and stiffness degradation. How this model is composed and what the influence of various parameters is on the global network response will be treated in more detail in chapter 4.

Note that various studies have specifically considered the progression of damage in lattice models: e.g., Delaplace et al. [40], Åström and Niskanen [41], Fleck and Qiu [42].
Table 3

<table>
<thead>
<tr>
<th>Width (mm)</th>
<th>Height (mm)</th>
<th>Experimental (kN/m)</th>
<th>Simulation (kN/m)</th>
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</thead>
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<tr>
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The tests on unnotched panels showed the presence of a size effect on the nominal strength, which was also explored through the model would have increased the variability of the numerical simulations and led to better agreement with the experiments.

The only significant difference between the experiments and the simulations was found in the scatter, which was taken into account in the simulations by using different network realizations but the models assumed that the interbundle friction (Fig. 11a) and the experimental results (Fig. 12) demonstrates, however, that the brittle fracture model cannot capture the tail of the curve and that interbundle friction plays a significant role in the localization of fracture in non-woven felts and, to a large extent, controls the total amount of energy dissipation.

Incorporating the damage process in accurate continuum models for paper, while limiting complexity, seems a daunting task. On the other hand, it appears that there is ample and surmountable room for improvement of the lattice modeling of paper’s in-plane mechanical behavior to failure. Therefore, considerations in the lattice modeling of paper are discussed in more detail in the subsequent chapter.

3.3 Discussion

In modeling paper using a continuum approach, much work has been done over the past decades. The elastic properties of paper have been extensively modeled, in which more and more mechanisms and details have been taken into account over time. In modeling the inelastic mechanical behavior of paper, it has been demonstrated that continuum models can be capable of simulating the in-plane mechanical response of paper realistically. Since continuum models do not straightforwardly deal with important inelastic effects in paper such as localization [9], they rely on rather non-trivial, phenomenological additions and fitting procedures in achieving a good agreement with experimentally obtained mechanical behavior. Therefore, it is concluded that continuum models of paper can be effective yet complicated.

On the other hand, few studies exist on the lattice modeling of paper (or similar materials). The available results show reasonable agreement with experimentally obtained behavior. A range of suggestions has been given on how to further improve these models. Despite the limited demonstrated capability of lattice models in simulating the mechanical behavior of paper, they are relatively simple means to do such. An important advantage of lattice models is that they allow naturally for the introduction of disorder [32]; damage and fracture at various locations can be modeled using moderate lattice sizes with fairly simple breaking rules for elements and bonds. The full capability of lattice models in simulating paper’s in-plane mechanical behavior remains yet to be demonstrated.

Incorporating the damage process in accurate continuum models for paper, while limiting complexity, seems a daunting task. On the other hand, it appears that there is ample and surmountable room for improvement of the lattice modeling of paper’s in-plane mechanical behavior to failure. Therefore, considerations in the lattice modeling of paper are discussed in more detail in the subsequent chapter.
3.3 Discussion
Chapter 4

Aspects of lattice modeling

In this chapter, considerations in setting up a lattice model are treated in section 4.1. Section 4.2 considers different methods found in the literature to model failure of fibers and to capture bond flexibility and failure in a lattice model in detail. Finally, section 4.3 discusses how the effective mechanical properties of a lattice can be determined.

4.1 Model composition

4.1.1 Dimensions

A choice that has profound consequences for results in modeling any material is the number of dimensions. Paper and similar fibrous materials are physically obviously three-dimensional, but to what extent can a two-dimensional lattice model accurately capture their behavior?

For many woven or knitted structures, the out-of-plane dimension plays a decisive role in the global response (e.g., transverse shear stress, bending effects), that is difficult to accurately simulate in two dimensions [35, 39, 43]. Such difficulties are also reflected in the fact that various analyses of woven structures are three-dimensional [44, 45], despite the enormous increase of the number of degrees of freedom (and thereby computational time) involved with the addition of a third model dimension [33].

For (glass-fiber) non-woven felts, it has been witnessed [39] that their piled-up fibrous structure keeps fiber motion confined to parallel planes, if it is assumed that the outward bending of external fibers has an insignificant impact on the in-plane behavior. In this case, it is assumed reasonable to simulate this material in two dimensions, by collapsing the contact problem through fitting normal forces (perpendicular to the model plane) that act on bonds.

Since paper has a planar fibrous microstructure that is remarkably similar to the glass-fiber non-woven felts considered by Ridruejo et al. [39], realistic results could be expected from the application of a similar model to paper. As is mentioned in section 3.2.1 however, Bronkhorst [9] has suggested three-dimensional modeling for paper to decouple network grammage from network density. Considering the extensive computational trouble of doing so, the present work will focus on laying a foundation for the full exploitation of two-dimensional modeling of paper: if this would turn out to be a dead end, the option of adding a third dimension can be examined in the future.

4.1.2 Element types and orientations

One important design aspect of a lattice model is the nature of the elements that connect the nodes. These elements may be either springs, trusses or beams [31]. Spring elements simply sim-
ulate a force interaction between two nodes, which is frequently used for the modeling of material interaction: e.g., Buxton et al. [46]. Trusses have a highly similar function. Beams, on the other hand, can transfer a moment of force, which makes them suitable for simulating objects with considerable bending stiffness; this is probably the reason that beams are commonly chosen in lattice models of (disordered) fibrous materials [1,9,39].

Alternative to linear spring elements, different (non-linear) constitutive behavior, including failure, could be prescribed for elements [47], as will be discussed in section 4.2.1.

A key property of a lattice in determining its effective mechanical behavior is the orientation of the elements; the inevitably limited number of element orientations in the network makes the lattice anisotropic. Isotropy can be approximated by choosing a very large number of randomly oriented identical elements or by using equilateral triangles. If few elements orientations are prescribed, for instance in a lattice with a high degree of periodicity, it is important to carefully choose the axes along which material behavior is evaluated.

4.1.3 Periodicity

In material modeling, introducing periodicity can reduce the complexity of the mathematics that are required to obtain solutions for a lattice model that is subjected to deformation. Periodicity can be employed on two levels; at the level of the lattice representation or at the level of a unit cell that contains a number of elements. These levels will be discussed in the sections below.

Our discussion is limited to two-dimensional lattice models as motivated in section 4.1.1, although three-dimensional lattice models of various types exist [1,48].

Representative Volume Elements

The first consideration is the actual representation of a lattice model. For some specific material samples, it might be necessary to capture the entire sample in a lattice in order to obtain realistic results. If, however, the introduction of degrees of symmetry in the model does not significantly affect the quality of results, the problem can be reduced to a representative volume element (RVE): i.e., a piece of material (‘element’) which has properties that are representative for the entire sample of material. Periodicity assumptions are often used to formulate the boundary conditions for such an RVE. The use of an RVE is common in modeling materials with a fibrous microstructure, since it allows for the identification of the influence of a range of morphological aspects on the mechanical behavior while limiting computational cost [1,9,31,39].

Periodicity in the lattice

Regardless of the ‘structure’ that the lattice represents (specific material sample or RVE), the lattice can be disordered or consist of (periodic) unit cells. These two types of lattice structures are discussed below.

A disordered lattice is characterized by a lack of order of the nodal positions: i.e., nodes are not arranged in a consistent pattern. Two-dimensional lattices have been applied to model randomly oriented fibrous materials by defining an RVE with a stochastic (disordered) arrangement of fibers [1,9,39], as shown in figure 3.6. Note that a disordered lattice may also be considered to be a Voronoi partitioning of the material domain of a continuum: e.g., of a two-phase material [33,49,50] as illustrated in figure 4.1.
As figure 4.1 illustrates, a material structure can be modeled explicitly through strategic grid point positioning. This gives disordered lattices an important advantage in dealing with for instance inclusions [50]. Other advantages are the ability to grade cell sizes to accurately capture local effects while saving computational expenses elsewhere, and performing adaptive mesh refinement in non-linear or time-dependent problems. A drawback of this approach is that local mechanical properties of the network (e.g., the Poisson ratio) may not be consistent or continuous in the model while they are in the actual material; such properties can therefore not be simply evaluated in great detail without additional treatment such as mesh refinement [50]. Important in modeling disordered fibrous materials such as paper is the adequate choice of topological properties of the defined lattice (e.g., distribution of fiber length, fiber orientation, fiber curl), since the effective mechanical properties strongly depend on these parameters [1]. The mechanical properties are usually determined by implementing the model in a finite element code which solves the displacement field. Usually, free fiber ends (that do not carry load) are removed before the simulation [1,39].

![Disordered lattice and the Voronoi tessellation it represents [50].](image)

On the other hand, nodes in a lattice might be defined in a periodic pattern. Such periodic lattices are characterized by a unit cell: i.e., a cluster of nodes and elements that repeats itself in the lattice space. Provided the properties of this unit cell are carefully chosen to adequately represent the material behavior, a periodic lattice can be applied to model continua or materials with a disordered morphology, like paper, in a convenient manner.

Although the introduction of a high degree of periodicity does not always reduce computational costs (since the number of structural elements is not necessarily reduced), it can introduce some degree of consistency in the mathematics that describe the lattice mechanics. The possibilities in composing and solving these mathematics are discussed in section 4.3. Another advantage of the high degree of periodicity is the consistency of local mechanical properties. A drawback may be that heterogeneities are not intrinsically incorporated in the lattice geometry. This may require the incorporation of features in the elements or nodes to simulate local failure, which is discussed in section 4.2. Furthermore, the smallest detail that is to be accurately captured in the periodic model determines the intricacy of the entire model. This may result in excessive computational costs due to mesh refinement in areas where it does not improve the results. Measures to avoid this are discussed in section 4.3.

Various distinct configurations of strictly ordered unit cells have been encountered in the literature; some of the most commonly used cells are depicted in figure 4.2. As discussed above, the number of element orientations in each cell strongly determines the anisotropy of the network. If elements represent fibers in materials such as paper, element orientations are referred to as discretized fiber orientations. A key feature in the lattice response is element connectivity [51]:
i.e., the number of elements connected to each node in a highly periodic lattice. Table 4.1 indicates these values for the five popular unit cell configurations that are considered here. Another mentioned characteristic is if a configuration is dominated by stretching or bending [51]. Table 4.1 also indicates how sensitive, according to Romijn and Fleck [51], the configurations are to nodal dispersion: i.e., how strongly some properties (in this case, the in-plane modulus and fracture toughness) are affected by random dispersion of joint positions from those of a perfect lattice.

A supplementary discussion of some aspects of certain configurations:

- **Triangular:** Approximates isotropic material behavior if equilateral: i.e., if internal angle $\theta = 60^\circ$ [52]. In simulating the elastic properties of paper, reasonable agreement with experimental results can be achieved for $45^\circ \leq \theta \leq 55^\circ$. The Poisson ratio and the ratio between the in-plane shear modulus and the Young’s modulus in MD are both inaccurate.

- **Square:** Transition cases [51]; the response can be bending or stretching dominated, depending upon the level of imperfection and upon the loading direction in relation to the microstructure for the square lattices. Structure has no intrinsic torsional stiffness; this can be overcome by using beam elements and prescribing rotational stiffness in the bonds, or alternatively by introducing an x-bracing.

- **Square x-braced:** Diagonal elements (x-brace) are introduced to give the structure shear stiffness, even when using trusses and bonds that are free of rotation stiffness. A fifth node may be included that connects the two diagonal elements in the middle of the cell [52]. Optimal simulation of paper’s elastic properties with internal angle $30^\circ \leq \theta \leq 40^\circ$. In this respect more suitable than triangular unit cell, since Poisson ratio and the ratio between the in-plane shear modulus and the Young’s modulus in MD are accurate for this unit cell.

- **Hexagonal:** ‘Honeycomb’ structure. The only unit cell listed here in which fibers are not modeled as running straight through the lattice.

- **Kagome:** Also referred to as a ‘Stars of David’ pattern. Bending or stretching domination depends on the level of imperfection [51].

### 4.1.4 Geometric relations in paper

The above sections have made clear that in the composition of lattice models for paper, various assumptions are made on morphological aspects: e.g., fiber distribution, curl characteristics, bond density per unit area. Some of these parameters are related to one another, but how? Various papers have been published over the past decades which study paper (or similar fibrous materials) on a geometrical level. These models are aimed at the derivation of relations between various geometrical features, such as free fiber length, bonding level and network density. Noticeable studies in this field are (chronologically) those by Kallmes et al. [4], Komori and Makishima [5], Deng and Dodson [6] and Niskanen [8].
4.2 Incorporation of component behavior

Breaking of the lattice is not a natural consequence of the simulation, as is the case in molecular dynamics, but has to be incorporated in the model as an additional behavior [32]. The following discusses the incorporation of fiber failure as well as bond flexibility and failure in lattice models, as found in the literature.

4.2.1 Fibers

A wide range of constitutive behavior can be prescribed for elements. By far the most common choice is linear elasticity; reasons for this may be that the modeled (fibrous) material is brittle and thereby elastic on the elemental scale [33, 39] and that the reversibility of elasticity allows for implementation without accounting for residual strains. Deviations from elastic behavior of a modeled material can be accounted for by using elements that can behave plastically [9, 47] and/or by simulation of plasticity in the bonds, which will be treated in section 4.2.2. In the modeling of materials that have been witnessed to be brittle on the elemental level (e.g., concrete, glass fiber), failure can be accounted for by changing an elastic element when its state (strain, stress, energy) meets a pre-defined criterion.

To simulate this elemental brittleness, a widely adopted approach is to perform quasi-static loading of a lattice (i.e., incrementally increased external loading of a lattice). For each loading level, a stable situation for subsequent loading is found by sequential removal of every element which violates a pre-defined threshold [33, 38, 53]. Equivalently to element removal, an element’s load-carrying capacity may also be set to zero [50]. The following sections discuss various thresholds that are found in the literature to determine if lattice elements experience brittle failure in quasi-static loading analyses.

Brittle tensile failure

One example of a paper that has applied this procedure to model element failure in a beam lattice has been published by Schlangen and Van Mier [49] and was later elaborated by Lilliu and Van Mier [33]. They have modeled the granular structure of a cement-based composite material. Their criterion is defined as a threshold for the effective axial beam stress $\sigma^*$ as follows:

$$\sigma^* = \frac{F}{A} + \alpha \sqrt{\frac{M_x^2 + M_y^2}{W}}$$  \hspace{1cm} (4.1)

In this expression, $A$ and $W$ are the area and the section modulus of the cross-section (for beams $A = bh$ and $W = bh^2/6$, where $b$ and $h$ are respectively the width and height of their cross-sections [49]) and $F$, $M_x$ and $M_y$ are the internal axial force and bending moments. A scaling...
factor $\alpha$ is introduced for the bending stress relative to the axial stress. Schlangen [54] has showed that small values of this factor give a long tail in the stress-deformation response. However, according to Tzschichholz [55], taking $\alpha = 0$ might lead to the occurrence of peeling effects in the fracture process in case of a rectangular lattice. A value commonly used in two-dimensional lattice simulations is $\alpha = 0.005$. Lilliu and Van Mier [33] have claimed that in their analysis, a variation of $\alpha$ in the range $0.00 \leq \alpha \leq 0.05$ would not affect the crack pattern. Various papers have applied the present theory to model lattice element failure: e.g., Bolander and Sukumar [50] and Liu et al. [38].

### Brittle tensile and shear failure

Heyden [1] has proposed a criterion for brittle failure of rectangular cross-section fiber beam elements that is a function of both normal stress and shear stress: a beam fails when $f(\sigma_n, \tau) = 0$, where $\sigma_n$ and $\tau$ are the respective maximum normal and shear stresses. These are specified as:

$$
\sigma_n = \pm \frac{N}{A_f} \pm \frac{M}{I_f} \sqrt{\frac{3I_f}{A_f}} \quad \tau = \frac{1.5V}{A_f}
$$

which uses the axial force $N$, bending moment $M$, shear force $V$, beam cross-sectional area $A_f$ and the corresponding moment of inertia $I_f$. Second-order effects like compressive stiffness decrease and buckling are not taken into account. For a two-dimensional (beam) lattice, the criterion is specified as:

$$
f(\sigma_n, \tau) = \max \left( \frac{|\sigma_n|}{\sigma_{ult}} - 1, \frac{|\tau|}{\tau_{ult}} - 1 \right)
$$

where the subscript $ult$ indicates the ultimate value (a threshold).

Heyden has evaluated the influence of fiber failure on the mechanical response of a rigidly bonded lattice of elastic beams that undergoes tensile tests. The stress-strain curve exhibits a sawtooth-like pattern, as is shown in figure 4.3; the occurrence of fiber failure causes both the global stress and strain of the entire network to repeatedly drop by noticeable amounts. The relative relapse in stress and strain seems to be approximately equal; this results in the radial character of the drops.

![Figure 4.3: Stress-strain response of a network that is dominated by fiber failure and lacks bond failure. [1]](image-url)
4.2 Incorporation of component behavior

Discussion

The presented tension-dependent fiber failure criterion by Schlangen and Van Mier [49] seems a straightforward way of implementing fiber failure, by bounding the axial stress. This is in agreement with observations that tension in fibers (together with bond shear) is the dominant mode of deformation in both two and three dimensions [56]. The effect of the scaling factor \( \alpha \) in the threshold stress on the network’s mechanical behavior might need further investigation. If, for a particular lattice, varying \( \alpha \) in the domain \( 0 \leq \alpha \leq 0.05 \) does not significantly affect the network response, in correspondence with the findings by Lilliu and Van Mier [33], one could prefer to choose \( \alpha = 0 \) for the sake of simplicity.

In addition to the axial beam stress criterion, Heyden also considered a shear stress criterion. If trusses or spring elements are used, this shear criterion is irrelevant; the problem then reduces to one similar to that presented by Schlangen and Van Mier [49]. The factor \( \alpha \) in (4.1) facilitates tuning of the importance of bending moments, and even allows for complete neglect of these bending moments which is done in various papers, whereas the bending moment contribution in the failure criterion by Heyden (4.2) is fixed for a certain set of parameters. Moreover, Heyden has not elucidated the origin of the criterion: e.g., from which assumptions it is derived, what the role of the \( \pm \)-operators is.

4.2.2 Bonds

A critical failure mechanism in the plastic behavior of paper [9, 30] (and other fibrous materials [39]) is the loss of inter-fiber connectivity. This failure can be induced by chemical bond failure accompanied and followed by inter-fiber sliding [1]. The importance of this mechanism is reflected in the fact that some network models even assume that all plastic deformation under tension occurs in the inter-fiber bonds while the fibers remain elastic [57]. In most papers, bonds are assumed to be deformed in a shearing mode [26]. Different explicit manners to model bond failure are found in the literature; some of the most relevant are discussed in this section.

Rigid and rigid-brittle bonds

In a recent paper, Liu et al. [38] have modeled paper using a two-dimensional periodic Timoshenko elastic beam lattice that included rigid-brittle bonds. In the used Kagome lattice (see figure 4.2), every node connects the ends of two pairs of aligned elements, so four fiber ends in total. The article considers pairs of aligned fibers to represent a part of a continuous fiber; some elements are removed to prevent fibers from being modeled as continuous throughout the entire lattice. If the connection (bond) between two continuous fibers (i.e., four element ends) is modeled as one node, the authors have argued that failure of the inter-fiber connection involves nodal splitting, that would require some special numerical techniques to handle the increasing number of nodes involved with lattice failure. To overcome this issue, they have modeled the connections of two pairs of aligned fiber ends as two nodes in the same point (each connecting two fiber ends), which are separated when the node shear stress meets the following criterion:

\[
|\tau| = \frac{|q|}{A_b} = \tau_c \tag{4.4}
\]

where \( \tau \) appears to be the average bond shear stress (not defined in the article), \( q \) is an effective inter-fiber connection force defined as the ‘shearing interaction’ between two fibers, \( A_b \) is the bond area and \( \tau_c \) is assumed to be the critical bond shear stress. For the Kagome lattice, it is argued that the angle between two fibers is \( \pi/3 \) such that \( A_b = 2h^2/\sqrt{3} \). For the unconstrained bonds (i.e., the bonds that are allowed to experience failure), the shearing interaction is defined as a product of the normal forces \( N_i \) and perpendicular ‘shear’ forces \( Q_i \) of the ends of the two aligned
elements \((i = 1, 2)\), experienced from the connected aligned element pair (fiber) as illustrated in figure 4.4, according to:

\[
|q| = \sqrt{(N_1 + N_2)^2 + (Q_1 + Q_2)^2}
\]  

(4.5)

Figure 4.4: Illustration of the normal forces \(N\) and tangential forces \(T\) on the fiber ends in the paper model by Liu et al. [38].

The critical shear stress is specified in the paper as follows:

\[
\tau_c = \theta \epsilon_{\text{max}} \sqrt{\frac{t}{h}}
\]  

(4.6)

where \(\epsilon_{\text{max}}\) is the strain at which the paper fails and thereby exhibits a steep drop in the stress-strain curve (observed values for paper \(0.2\% - 1.2\% [2,28,41]\)) and \(\theta\) is an adjusting factor. When the shear criterion (4.4) is met, the pair of unconstrained bonds is split into two separate bonds, each connecting two aligned element ends, thereby forming two separate fibers. These two separated bonds are then regarded as constrained: i.e., they are rigid and thereby cannot experience failure.

The element thickness in the two-dimensional lattice is characterized as one of the highest measured values of paper thickness. The lattice elements therefore represent fiber bundles. The element aspect ratio \(h/t\) is claimed to be critical in giving the Poisson ratio \(\nu\) a meaningful value (Isaksson and Hägglund [28] have suggested \(\nu = 0.29\); Liu et al. have taken \(\nu = 0.25\) and \(h/t \approx 0.38\)). In the choice for the fiber and bond strengths, the authors have argued that in a linear elastic lattice as the one that they use, the shape of the force-displacement curve is not influenced by the absolute value of the strength limit itself, but by the ratio of fiber strength to bond strength. For a fixed bond strength, simulations are performed for various fiber strengths ranging from values that make the fibers either considerably weaker than the bonds, or much stronger, or the strengths of fibers and bonds are such that they both fail. The strengths chosen to let both bonds and fibers fail are considered to be a lower bound of reality; for the fibers this is attributed to the lack of plasticity and fiber curling in the model and the bonds are considered to fail more easily due to an overestimation of the fiber thickness in the two-dimensional plane. The authors have emphasized that the strength values have been chosen in a rough manner, since they expect their study to give only qualitative results.

The predicted stress-strain curves typically show initial linear elastic behavior followed by slight yielding while failure is scattered; failure is monitored during the quasi-static (incremental) loading procedure. If a failure band emerges and extends, the network suddenly loses its load-carrying capacity, reflected by a drop in the stress-strain response. This physical process appears to be in agreement with that simulated by Åström and Niskani [41]. For subsequent straining relatively low and (approximately) constant stresses are measured. Liu et al. have qualitatively identified the influence of some properties on this mechanical behavior. For instance, increasing the fiber length (aspect ratio) causes the stiffness, strength and toughness to increase while the width of the failure bands also increases. The fiber-to-bond strength ratio does not affect the stiffness but only
the strain at which failure occurs is increased with this ratio, while the failure band is narrowed.

Anisotropic elastic bonds with stepwise failure
To capture various fiber interaction mechanisms - such as interlocking, friction and chemical bonding - that are witnessed in fluffed dry-shaped cellulose fiber materials, Heyden [1] has proposed fictive bond elements. These materials are modeled as networks of Bernoulli beams in two and three dimensions. A bond is modeled as two circular plates with area $A_b$ connected by distributed springs, as illustrated in figure 4.5. The circular areas are rigidly connected to the fiber center lines, perpendicular to the line connecting the two fiber center lines at the bond location and at zero distance from each other. Under loading, a bond shows a stepwise-linear stick-slip behavior: bond stiffness and strength properties are degraded when a slip criterion $g = 0$ is fulfilled, where $g$ is a (dimensionless) function of the loading conditions. The number of times the criterion can be met until bonds fail completely is set by a parameter $n_s$.

![Figure 4.5: Bond for three-dimensional models proposed by Heyden, depicted in two dimensions. Note that the bond has stiffness $k_1$ in the dimension perpendicular to both dimensions of the figure [1].](image)

![Figure 4.6: Schematic of a one-dimensional bond for two-dimensional models proposed by Heyden [1].](image)

For the springs in between the plates, two models have been suggested: ‘coupled springs’ and ‘uncoupled springs’. In the coupled springs version, the bond has a normal stiffness $k_n$ and a shear stiffness $k_t$ in all directions perpendicular to the normal direction. A dimensionless bond loading function $g$ can now be expressed in terms of the average normal stress $\sigma_n$ and shear stress $\tau$ in the bond as follows:

$$g(\sigma_n, \tau) = \frac{|\tau|}{\mu(\sigma_{adh} - \sigma_n)} - 1$$  \hspace{1cm} (4.7)

where $\sigma_{adh}$ represents the adhesion strength and $\mu$ is a shear strength factor. If $g(\sigma_n, \tau) = 0$ is met under compressive normal stress ($\sigma_n < 0$), the bond stiffness degradation is specified as applying correction factors $\lambda_1$ to $k_t$, $\lambda_2$ to $\mu$ and $\lambda_3$ to $\sigma_{adh}$. These correction factors determine the amount of degradation in the corresponding bond parameters. When the slip criterion is fulfilled
under tensile normal stress ($\sigma_n > 0$), the bond is assumed to experience complete fracture; this is equivalent to taking $n_s = 1$. When modeling in two dimensions, the mode of deformation which separates the circular areas is irrelevant; hence, only the shear springs are present so $\sigma_n = 0$ in (4.7). In this case, the tangential stiffness could be further specified as two translational stiffnesses $k_x$ and $k_y$, and a rotational stiffness $k_\phi$; due to the two-dimensional modeling, the bond can then be regarded as a (one-dimensional) series of three uncoupled springs, shown in figure 4.6. In the slip criterion, a distinction is made in this case between shear stresses induced by forces and by moments, resulting in the following expression:

$$g(F, M) = \frac{|F|}{F_{ult}} + \frac{|M|}{M_{ult}} - 1$$

where $|F|$ is the norm of the vector sum of the forces experiencing translational stiffnesses, $F_{ult}$ is the ultimate force of the bond, $|M|$ is the norm of the moment experiencing rotational stiffness and $M_{ult}$ is the ultimate moment of the bond. It appears that if the criterion is met, stiffnesses $k_x$, $k_y$, and $k_\phi$ are corrected by factors $\lambda_1$ and strengths $F_{ult}$ and $M_{ult}$ are corrected by a factor $\lambda_2$, as is illustrated in figure 4.7 for $F_x(u_x)$. Again, $n_s$ dictates the number of times the criterion can be met until complete bond failure. It is noted that the effects of fiber slip and new bond formation in a changed configuration remain to be accounted for.

The mechanical response of a network of strong fibers and bonds that are prone to failure is evaluated. Just like for pure fiber failure networks (see section 4.2.1), bond failure gives the stress-strain curves a sawtooth-like pattern in radial direction with respect to the origin. A noticeable difference is that the jumps are more numerous and intricate for the bond failure network than for the fiber failure network. This is explained by the fact that the failure of a bond has a less profound influence on the load-carrying capacity of the network than the removal of a fiber, which destroys an entire load path. The influence of various bond properties on this bond failure dominated network response is identified as follows:

- An increase of the bond strength proportionally increases both stresses and strains of the network’s mechanical response curve.
- An increase of the bond stiffness (i.e., all $k_x$, $k_y$ and $k_\phi$) increases the network stiffness and decreases the overall stresses and strains. These relations appear to be non-linear. Network stress levels seem less strongly dependent on the bond stiffness than on the bond strength for the considered set of values.
• Global network stresses and strains increase with \( n_s \) (maximum stress increases linearly with \( n_s \)), due to increased strain redistribution

**Isotropic frictional bonds**

Based on their experimental observations, Ridruejo *et al.* [39] have recently implemented a frictional stick-slip model in a two-dimensional non-periodic Timoshenko beam lattice that represents a non-woven felt of glass-fiber bundles. The resultant tangential bond forces \( T \), inter-fiber friction coefficient \( \mu \) and normal force of contacting fiber bundles \( N \) (which is perpendicular to the network plane) are captured in a ‘pseudopotential’ \( \Phi \) (in unit of force), defined as:

\[
\Phi = T - \mu N
\] (4.9)

As long as the tangential forces do not exceed the frictional forces (i.e., \( \Phi \leq 0 \)), the bond is assumed to be linear elastic. Its stiffness is computed from the shear modulus of a ‘binder’; a material which is assumed to bind two fiber bundles over an area \( h^2 \) and thickness \( h/5 \), where \( h \) is the fiber bundle thickness. If the tangential forces exceed the frictional forces (\( \Phi > 0 \)), sliding occurs and this motion is penalized by a friction force \( \mu N \). This penalization is modeled in a phenomenological manner, described by a bi-linear decay function \( N(\delta) \), as shown in figure 4.8. Its peak (starting) value is dictated by the critical tangential force \( T_{\text{crit}} \): i.e., the tangential force corresponding to slip initiation \( \Phi = 0 \), according to \( N(\delta = 0) = T_{\text{crit}}/\mu \). The displacements that indicate the onset and end of the second linear regime and the stiffnesses of both regimes are not experimentally determined, but used as fitting parameters for the friction-dominated region of the nominal stress-strain curves. This friction implies energy dissipation; the integral of \( N(\delta) \) over \( \delta \) is a measure for the amount of energy dissipated in a bond until ‘full pullout’ (i.e., complete separation of two fibers) is reached.

![Figure 4.8: Bilinear decay of the normal bond stress \( N \) as a function of sliding displacement \( \delta \) for \( \Phi > 0 \) [39].](image)

The authors claim that the bond behavior may be captured in many alternative models other than the frictional stick-slip bond model; an elastic-brittle bond model, where the bond is linear elastic until complete failure, is also used for the sake of simplicity. The authors claim that the bond failure model they suggest is the first that includes the influence of friction on the mechanical response.

The stress-strain curves of lattice simulations using the frictional stick-slip bonds are compared to those using elastic-brittle bonds. It is illustrated that the initial elasticity is hardly affected by the bond model; the only difference is that the frictional bond model yields some ‘dents’ or brief
4.2 Incorporation of component behavior

stress drops in the (approximately) elastic regime, whereas the elastic-brittle bonded lattice results in a more smooth near-linear curve. As failure sets in and the stress peaks, the elastic-brittle bond model results in an abrupt drop in stress (that corresponds to lattice failure) followed by a near-zero erratic stress pattern. On the other hand, with the frictional bond model, a somewhat higher strength is achieved, the post-peak drop in stress is less dramatic and it is followed by a much more gradual loss of load-carrying capacity of the lattice. An energy-strain graph demonstrates that this is due to dissipation of elastic energy by the bond friction. In another diagram, shown in figure 3.8, the stress-strain curves of three lattice simulations using frictional bonds are plotted over the feasible domains of experimentally found mechanical behavior. Using fixed averages of observed parameter values for the simulations, the stiffness and strength cannot be fitted, while the characteristics of the bond normal force decay are used as fitting parameters for the softening portions of the curves. The simulated results are shown to be in fair agreement with the approximate average experimentally found mechanical behavior; the elastic portions are nearly identical (apart from some roughness in the numerical curve) whereas in the peak and softening portions of the curves there is much scatter in the results of the three simulations, involving ~ 50% variations. Still, the results are well within the limits of the experimental data, which show even more scatter. This scatter is attributed to variations in both network geometry and inter-bundle strength that are absent in the simulations. Incorporation of these variabilities in the numerical models is firmly predicted to lead to a better agreement with experimental results.

Discussion

The model with rigid and rigid-brittle bonds presented by Liu et al. [38] is a seemingly computationally efficient way to obtain qualitative insights in the scaling relations of a paper-based lattice model. The influences of the fiber aspect ratio and the fiber to bond strength ratio on the mechanical behavior are illustrative, as are the identified pitfalls of leaving out plasticity and fiber curl and poorly estimating fiber thickness. Unfortunately, various choices for model composition and for parameter settings tend to lack explanation and/or seem rather ad hoc, even for a qualitative model. The choice for elastic elements with uniform properties is not motivated beyond simplicity, neither is the choice for rigid-brittle bonds. Bending moments in the fiber failure criterion are disregarded after the notification that this is done in a lattice model for concrete, despite that it is not the usual approach in modeling. Moreover, the accuracy of such features and parameter choices in simulating paper’s mechanical behavior, which could have been evaluated by comparing simulation results to experimental observations, largely remains a guess.

Heyden [1] has presented extensive elastic bond models; their applicability to both two and three dimensions, tunable stiffness and strength decay, variable ductility and anisotropic characteristics makes these bond models versatile. Although the relevance of modeling anisotropy is not clarified, the presented influences of bond stiffness, strength and ductility on a bond failure dominated network response are informative. As the author has noted, a potentially considerable limitation of the bond model could be the lack of incorporating the effects of fiber sliding in the bonds, such as energy dissipation by friction.

A lattice model that incorporates energy dissipation in the bonds is that for non-woven glass fiber felts as presented by Ridruejo et al. [39]. A (bilinear) sliding resistance decay is defined, that allows the network response to qualitatively match the experimentally determined response in the softening-pullout regime, which is dominated by (localized) bond failure. By quantitatively fitting the bond energy dissipation to the experimental response, the fitted results seem reproducibly well within the limits set by experiments. Additional information is needed to validate this model more accurately, and questions arise on the suitability of the bilinear and other bond characteristics in accurately simulating the mechanical behavior of other fibrous materials with a stochastic microstructure, such as paper. The authors’ claim, that the use of homogenous bond strengths (and lattice spacings) limits the accuracy of simulation of the considerable scatter that
is witnessed in experimental stress-strain data, is yet to be proven.

4.3 Solution methods

Obtaining the effective macroscopic mechanical behavior of a defined lattice is done by composing a mathematical system that describes the network (for periodic networks through the unit cell) and subsequently solving it: i.e., obtaining a displacement field which corresponds to the lattice being in a state of equilibrium. Methods for solving one- and two-dimensional configurations and various element types have been proposed in the literature; Ostoja-Starzewski [31] has presented a detailed overview to this end. Some clear examples of solutions for two-dimensional lattices that can be used to model materials with a disordered topology are treated here.

A dissipation-free lattice of springs can be solved by means of the potential energy minimization approach [50, 58]. This method makes use of the fact that the total potential energy of a lattice is minimal if it is in a state of equilibrium. First, the nodal energies are expressed as half of the adjacent truss potential energies. The total internal potential energy of the lattice is the sum of these nodal energies. If the external potential energy (i.e., the potential work done by body forces) is subtracted, the result is the total potential energy of the lattice. The displacement field that minimizes this total potential energy is the solution; this minimizer can for instance be found using classical variational principles and Newton-Raphson. With the solution, the overall stiffness matrix can be determined.

The truss potential energy can also be used to derive the effective continuum properties of a unit cell in a spring network model [31]. This method relies on the equivalence of strain energy stored in the elements of a unit cell $U_{cell}$ and the strain energy that would be stored in the (fictional) piece of continuum that the unit cell represents, $U_{continuum}$. The equivalence $U_{cell} = U_{continuum}$ can be expressed as:

$$\sum_{e} \frac{1}{2} (F \cdot u)^e = \int_{V} \frac{1}{2} \sigma \cdot \epsilon dV$$

(4.10)

where $e$ indicates an element-wise counting, $N_e$ is the number of elements, $F$ and $u$ are the respective force and generalized spring displacement, and $\sigma$ and $\epsilon$ are the stress and strain in the continuum respectively. When using linear elastic elements (stiffness $k$), spatially linear displacement fields and analyzing in two dimensions, the balance can be written as:

$$\sum_{e} \frac{1}{2} (k u \cdot u)^e = \frac{1}{2} \epsilon \cdot C \cdot \epsilon$$

(4.11)

From the choice of the unit cell and type of interactions, a connection can be made between $u$ and $\epsilon$, and $C$ can be derived from (4.11). Examples of how the elastic properties of square and triangular network geometries can be derived using this method are given in [31].

The elements of the lattice can also be regarded as trusses or beams instead of springs. In these cases, the effective mechanical properties of a unit cell (e.g., moduli, Poisson’s ratio) can be obtained by solving a system of force equilibria for all the nodes every dimension [52]. Note that the displacement solution of a spring lattice can also be obtained by solving force equilibria. Derivation of the effective elastic properties of triangular and x-braced square unit cells using force equilibria are given in [52].

Note that solving lattices can be computationally expensive [58]. The smallest detail that is to be accurately captured in the model determines the intricacy of the entire model; when modeling
samples of considerable proportions with respect to the desired element size, the lattice can contain a considerable number of elements. This makes direct application of a lattice computationally inefficient. To overcome this obstacle, (multiscale) methods have been developed to reduce the computational costs while still allowing for detailed material modeling using lattices, such as the quasicontinuum method [58–60].
Chapter 5

Concluding remarks

As is explained in the introduction, a convenient and accurate model to predict the mechanical behavior of paper until failure would be welcome.

To have clearly in mind what to model, chapter 2 has shown that paper consists of a bonded fibrous network. When subjected to straining, the fibers and bonds that form the network initially exhibit elastic deformation. This is followed by elastic-plastic behavior, as the fibers (and perhaps the bonds too) gradually start to deform plastically and some bonds that are spread across the network experience failure of their chemical interaction. At some point, localization marks the onset of fracture; the fracture process is primarily characterized by bond failure, although fiber failure may also occur to a limited extent. When a fiber’s chemical connections have failed, the pullout of the connected fiber is resisted by frictional sliding of the fibers over each other, which is reflected in a tail in the stress-strain response.

Chapter 3 has presented an inventory of models that were used to predict the mechanical behavior of paper. It appears that many continuum models are available, that have been demonstrated to accurately model paper’s in-plane mechanical behavior to failure well. A drawback is that considerable complexity is involved with such a high level of accuracy. Lattice models have appeared to be relatively straightforward means of modeling paper, which naturally allow for the incorporation of disorder that is imminently present in paper’s fibrous microstructure. Their capability in accurately modeling paper remains yet to be fully demonstrated, and many openings for future research to this end exist.

Lattice models are therefore discussed in more detail in chapter 4. To predict the in-plane tensile behavior of paper, a two-dimensional lattice with a high degree of periodicity seems a good starting point, in which the element properties can be tailored to phenomenological behavior. Elastic elements can be chosen for simplicity, but considering the constitutive behavior of the fibers (and bonds) in paper, elastic-plastic behavior seems the optimal choice. To realistically simulate damage and fracture of the network, it is important to incorporate fiber failure and (especially) bond failure. Fiber failure has been incorporated in several lattice models, but achievements are limited in modeling bonds that initially have a strong (chemical) connection that can experience failure at a certain (shear) stress level, and which is followed by frictional sliding during fiber pullout that involves energy dissipation. Ridruejo et al. [39] recently incorporated such bonds in a lattice model of a glass-fiber non-woven felt with promising results, but left room for further research in the application of such a model to accurately describe the response of paper. Solution methods for lattices may have to be developed specifically to capture energy dissipation in the bonds.
Bibliography


