BiMaC Innovation Stage 4

The proposed research activities within Stage 4 are divided into five work packages (WP), as shown in Figure 1. Each work package consists of several activities, where at least two competence areas are involved.

Competence building research

The basic idea in Stage 4 is that PhD students will work within competence-building research activities. Hence, all PhD students that are currently enrolled in BiMaC Innovation will be engaged in 1 or 2 projects.

Implementation projects

Implementation projects that are used to increase the TRLs of the projects will be run. These will be performed by senior researchers and/or as in-kind activities by the partners. The expectation is that the partner companies will contribute heavily to these projects. It is important that the project can access relevant pilot facilities and characterization labs.

Figure 1. BiMaC Innovation consists of four proposed work packages, and their relations to the competence areas.
Project leaders for the implementation projects

**AMOR**: Katarina Jonasson, Tetra Pak

**3D-tool**: Mikael Nygårds, Innventia

**BioComp**: Lars Berglund, KTH

**AdHemi**: Jörg Brücher, Holmen

**Foam**: Lars Wågberg and Sören Östlund, KTH

Personnel

**Prashanth Srinivasa** has joined BiMaC Innovation as a graduate student in the Department of Solid Mechanics. He works on the analysis of the mechanical properties of CNF foams using numerical modelling, tomography scans and biaxial experiments under the supervision of Assoc. Prof. Artem Kulachenko.

Fangxin Zou is since September 1st, 2016, employed as a Post-Doctoral student. Fangxin’s project is about preparing low density materials from CNFs for use in packaging applications. Fangxin’s supervisor is Prof. Lars Wågberg and co-supervisor is Dr Per Larsson.

**Ran Bi** has a PhD from KTH and is since Oct 10th, 2016, working as a researcher in BiMaC Innovation. She is working together with Per Larsson and Verónica López Durán in the implementation project AMOR in the scale-up of the AMOR process.
Doctoral dissertations
Anton Hagman
Influence of inhomogeneities on the tensile and compressive mechanical properties of paperboard

Abstract
The in-plane properties of paperboard have always been of interest to paper scientists. Tensile properties are crucial when the board is fed through converting machines at high speeds. Compressive properties are essential in the later use. Inhomogeneities affect both the compressive and tensile properties. For the tensile properties, it is the inherent heterogeneity of the paperboard that might cause problems for the board-maker. Varying material properties, through the thickness of the paperboard, are on the other hand used to achieve high bending stiffness with low fiber usage. It is of interest to know how this practice affects the local compressive properties. Papers A and B aims to address this, while C, D and E focus on in-plane heterogeneities. Paper A investigates the mechanism that causes failure in the short span compression test (SCT). It was concluded that the main mechanism for failure in SCT is delamination due to shear damage. In paper B the effect of the through-thickness profiles on the local compression strength was examined. It was concluded that the local compression is governed by in-plane slippages and through thickness delamination. The latter was in turn dependent on the local shear strength and in-plane stiffness gradients. In paper C the tensile test is investigated with focus on sample size and strain distributions. The strain behavior was dependent on the length to width ratio of the sample and was caused by m:Liveiation of local zones with high strainability. Paper D focuses on the strain zones seen in C. The thermal response in paper was studied. It was observed that an inhomogeneous deformation pattern arose in the paper samples during tensile testing, it was concluded that the heat patterns observed coincident with the deformation patterns. It could be shown that the formation was the cause of the inhomogeneous deformation. In final paper, E, Yirual field method was applied on data from C.
Svetlana Borodulina
Micromechanics of fiber networks

Abstract

The current trends in papermaking involve, but are not limited to, maintaining the dry strength of paper material at a reduced cost. Since any small changes in the process affect several factors at once, it is difficult to relate the exact impact of these changes promptly. Hence, the detailed models of the network level of a dry sheet have to be studied extensively in order to attain the infinitesimal changes in the final product. In Paper A, we have investigated a relation between micromechanical processes and the stress-strain curve of a dry fiber network during tensile loading. The impact of "non-traditional" bonding parameters, such as compliance of bonding regions, work of separation and the actual number of effective bonds, is discussed. We conclude that large local strains are the precursors of bond failures and not the other way around. We attributed the overestimated network strength, as compared to experimental curves, to the overestimated number of contacts and other contact parameters. In Paper B, we studied the impact of the chemical composition of the fiber cell wall, as well as its geometrical properties, on the fiber mechanical properties using the three-dimensional model of a fiber with helical orientation of microfibrils at a range of different microfibril angles (MFA). We found that the shape of the fiber cross-section does not affect its tensile response significantly, as long as the area of the cross-section and the average MFA of the fiber are preserved. In order to accurately characterize the fiber and bond properties inside the network, via statistical distributions, microtomography studies on the handsheets have been carried out. This work is divided into two parts: Paper C, which describes the methods of data acquisition and Paper D, where we discuss the extracted data. Here, all measurements were performed at a fiber level, providing data on the fiber width distribution, width-to-height ratio of isotropically oriented fibers and contact density. We confirm that the number of fiber-to-fiber contacts in three-dimensional isotropic networks is controlled by the fiber's aspect ratio. In the last paper, we utilize data thus obtained in conjunction with fiber morphology data from Papers C and D to update the network generation algorithm in order to produce more realistic fiber networks. We also successfully verified the models with the help of experimental results from dry sheets tested under uniaxial tensile tests. Further on, we carry out numerical simulations on these networks to ascertain the influence of fiber and bond parameters on the network strength properties. We conclude, among other things, that it is sufficient to account for the average bond strength value with an acceptable number of samples to describe the dry network strength.
Mohd Farhan Ansari
Nanostructured Cellulose Biocomposites: Effects from dispersion, network and interface

Abstract
The major load bearing component in native wood, cellulose nanofibrils, are potential candidates for use as reinforcement in polymer matrices. This study is based on nanocellulose composites and attempts to prepare and characterize biocomposites with high nanocellulose content and investigate the influence of nanostructure on macroscopic properties. In an initial study, effects from cellulose nanocrystal (CNC) dispersion on optical and mechanical properties of CNC composites are studied in a model system using polyvinylacetate (PVAc) as the polymer. CNC surface modification is used as an aid to improve dispersion, and nanocomposites with up to 20 wt% of modified and unmodified CNC are characterized. Strong influence of CNC as reinforcement and on polymer matrix characteristics were observed with well-dispersed CNCs, resulting in nanocomposites with significantly improved mechanical properties. In the subsequent parts, an impregnation-based processing strategy is used to prepare cellulose nanofibril (CNF) based thermoset (epoxy and unsaturated polyester) composites with high CNF content (15 - 50 vol%). Influence of CNF surface hydroxyls on epoxy curing is discussed. A mono-epoxy compound is used to confirm covalent epoxy/CNF reaction and the implications of this modification on mechanical properties of wet CNF network are illustrated. Mechanical properties of thermoset composites are characterized at different relative humidities to evaluate their hygromechanical stability. The role of the CNF-thermoset interface is investigated by comparing composites with epoxy and unsaturated polyester matrices. Unique effects due to the nanostructure of composites are discussed with respect to CNF dispersion, CNF network characteristics and CNF/matrix interface. Additionally, pulp fiber composites, where the fiber wall itself is impregnated with resin, are designed and differences between nanocellulose (nanoscale network) and pulp fibers (microscale diameter) as reinforcements are analyzed.

Master theses
Jonna Holmqvist
Hemicellulose-based wood adhesives

Abstract
The interest in producing alternatives to petroleum-based wood adhesives is due to the growing consciousness of fossil fuels’ impact on the environment. Also, the paper industry needs to adapt to a market where paper is replaced by technology, and develop new
materials and functions from wood. A wood adhesive is a material that chemically and/or physically binds two wood surfaces together. Today most adhesives are petroleum-based and the main application, volume-wise, is manufacturing building materials, such as plywood. Hemicellulose is a group of polysaccharides that reside within the cell wall of terrestrial plants. Hemicellulose is the second most abundant polysaccharide family in nature, after cellulose, and it is a hydrophilic component that contributes to the plant cell wall’s flexibility by linking together cellulose and lignin. Galactoglucomannan is the most common hemicellulose in softwood, while xylan is the most common hemicellulose in hardwood. In this study, hemicellulose has been used as a binder in adhesive mixtures. The hemicellulose was extracted using a pilot-scale model for pre-hydrolysis and sulfate cooking of hardwood and softwood wood chips at Holmen AB, to simulate the industrial process. Parameters that were evaluated were conditioning time (24 h and 7 days), different dispersing agents (PVAm, PEI and chitosan), different solid content of hemicellulose (20, 30, 40, and 50 wt%), different pH of dispersing agents, different strain rates (1 mm/min and 50 mm/min). A comparison between applying mixed components and applying the components separately has also been performed. The results showed that 20 and 30 wt% solid content in the adhesive gave the best result, PVAm directly from the bottle performed best as a dispersing agent and there was no significant difference between conditioning the samples 24 h and 7 days. Furthermore, mixing the components before application showed better results, and there was no large difference between 1 mm/min and 50 mm/min strain rate. The samples have been characterized using Fourier transform infrared spectroscopy (FTIR), and evaluated using Instron 5566 to determine the critical separation stress. The extracted hemicellulose was sent to MoRe Research for carbohydrate and molecular weight analyses.

Publications

Eric Linvill and Sören Östlund
“Biaxial In-Plane Yield and Failure of Paperboard”

Abstract
Paperboard is oftentimes subjected to biaxial in-plane stress and strain states, although very few experimental studies of the biaxial in-plane yield and failure of paperboard have been conducted. A new biaxial testing method to determine the in-plane stress- and strain-based yield and failure surface of paperboard was proposed and implemented. The method utilized cruciform specimens containing a reduced-thickness region (prepared by laser engraver) to increase probability of failure in that region, and digital image correlation was utilized to measure strain. The obtained stress-based failure surface was similar to previously reported results in the literature, but the obtained strain-based failure surface differed from the one previously reported strain-based failure surface. The obtained yield and failure sur-
faces had similar shape, providing confidence in both results due to the related deformation and failure mechanisms in paperboard. Furthermore, the overall shape of the stress- and strain-based yield surfaces was unaffected by the definition of the yield point. The obtained strain-based failure surface revealed the forming limits and therefore strengths and limitations of various 3-D forming methods for paperboard.

Prashanth Srinivasa, Artem Kulachenko and Filip Karlberg
“Material properties of the cell walls in nanofibrillar cellulose foams from finite element modelling of tomography scans”
Cellulose, under review.
Also available as a Master’s thesis by Filip Karlberg.

Abstract
Finite element simulations of artificially generated foam structures require the knowledge of the constituent solid mechanical properties. These are hard to determine directly from experiments because of the length scales involved. We combined reconstruction of X-ray tomography scans together with finite element simulations to determine the elasto-plastic material properties of the cell wall. To overcome the uncertainty introduced by thresholding in the reconstruction technique, the reconstructed structure was parametrized with respect to thresholding and thus relative density. Power law relations equivalent to scaling laws were fit to the results obtained from simulations of reconstructed structures. These were then extrapolated to obtain elastic modulus and yield strength of cell-wall material. In addition to the material properties, the simulations also corroborated the damage mechanisms in the compression of nanofibrillar cellulose foams. These insights together with the material properties will be used for studying representative abilities and scale effects of large artificially/numerically generated three-dimensional foam structures.
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