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Structure and hygroelastic properties of conifer branch wood

A multiscale approach

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ACTA UNIVERSITATIS
UPSALIENSIS
2024

ISSN 1651-6214
ISBN 978-91-513-2322-0
urn:nbn:se:uu:diva-543259

UPPSALA
UNIVERSITET

Dissertation presented at Uppsala University to be publicly examined in Polhemsalen, Ångströmlaboratoriet, Lägerhyddsvägen 1, Uppsala, Friday, 24 January 2025 at 09:25 for the degree of Doctor of Philosophy. The examination will be conducted in English. Faculty examiner: Dr. Michaela Eder (Max Planck Institute of Colloids and Interfaces).

Abstract

Hartwig-Nair, M. 2024. Structure and hygroelastic properties of conifer branch wood. A multiscale approach. *Digital Comprehensive Summaries of Uppsala Dissertations from the Faculty of Science and Technology* 2478. 37 pp. Uppsala: Acta Universitatis Upsaliensis. ISBN 978-91-513-2322-0.

Studies of structure-property relationship of compression (CW) and opposite wood (OW) formed in conifer branches are rare, mostly due to their lack of application in construction. Instead most branch wood is today being used as fuel. However, utilising branches as material can contribute to a more efficient and sustainable use of forest biomass and reduce the demand of stem wood for engineered wood products. Furthermore, deeper insight in compression and opposite wood might inspire toward new engineering solutions by using principles prevalent in the tree branch.

This thesis investigates hygroelastic properties of compression and opposite wood in branches by modelling and experimental techniques at several hierarchical material levels.

First, mechanical optimisation of tree branches for bending by using compression and opposite wood in a beam model is analysed. One weakness of the analytical model is the lack of elastic properties of compression and opposite wood of branches. Hence, hygroelastic properties for these are determined by mechanical testing and micro-computed tomography.

Following that, swelling behaviour of CW and OW lignin is studied by Molecular Dynamics (MD) simulations and wide-angle X-ray scattering to understand the effect of their chemically distinct structure.

Lastly, a hierarchical multiscale model is established to study the effect of previously determined lignin swelling coefficient, as well as lignin content and microfibril angle on swelling properties of cell walls. Swelling coefficients and elastic properties obtained by MD simulations are used as an input for Finite Element modelling.

The branches composition of compression wood and a opposite wood indicates that it is optimised for bending resistance. The hygroelastic properties of the comprising tissues are obtained. The swelling of CW is much less anisotropic than CW. The structural differences in lignin of compression and opposite wood and their resulting different swelling coefficient do not lead to different swelling of the compression and opposite wood cell walls.

The experimental and modelling approaches in this thesis are not specific to branch wood and can be of interest in wood science in general to gain more insight into the effect of structural changes on moisture-wood interaction and hygroelastic properties.

Keywords: compression wood, opposite wood, reaction wood, hierarchy, swelling

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ISSN 1651-6214
ISBN 978-91-513-2322-0
URN urn:nbn:se:uu:diva-543259 (http://urn.kb.se/resolve?urn=urn:nbn:se:uu:diva-543259)

Dedicated to my family

List of papers

This thesis is based on the following papers, which are referred to in the text by their Roman numerals.

I Hartwig-Nair, M., Gamstedt, E. K., Florisson, S., & Wohlert, M. (2024). Softwood branches modelled as a composite beam of compression and opposite wood: investigation of bending resistance. *Wood Material Science & Engineering*, 19(4), 979-986.

II Hartwig-Nair, M., Florisson, S., Wohlert, M. & Gamstedt, E. K. (2024). Characterisation of hygroelastic properties of compression and opposite wood found in branches of Norway spruce. *Wood Science & Technology*, 58, 887-906.

III Hartwig-Nair, M., Nasedkin, A., Hackenstrass, K., De Santis, E., Florisson, S. & Wohlert, M. Lignin Hygroexpansion in Compression and Opposite Wood - a Molecular Dynamics study. *Under Review at Wood Science & Technology.*

IV Hartwig-Nair, M., Andriani, F., Tabudlong Jonasson, N., Karlsson, M., Rosén, T., Florisson, S., Gamstedt, E. K., Lawoko, M. & Wohlert, M. Structural analysis of compression and opposite wood lignin by X-ray scattering and molecular dynamics simulations. *Manuscript.*

V Hartwig-Nair, M., Florisson, S., Wohlert, M. & Gamstedt, E. K. Modelling Hygroexpansion of Compression and Opposite Wood of Conifer Branches - Bridging the Gap between Molecular and Cell Wall Level. *Manuscript.*

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Author’s contribution

I. Conceptualisation, Methodology, Visualisation, Writing -Original Draft

II. Conceptualisation, Investigation, Formal analysis, Visualisation, Writing -Original Draft

III. Conceptualisation, Writing - Review & Editing

IV. Conceptualisation, Investigation, Formal analysis, Writing - Original Draft

V. Conceptualisation, Methodology, Visualisation, Writing -Original Draft

Papers not included in this thesis

i. Florisson, S., Hartwig, M., Wohlert, M. & Gamstedt, E. K. (2023). Microscopic computed tomography aided finite element modelling as a methodology to estimate hygroexpansion coefficients of wood: a case study on opposite and compression wood in softwood branches. *Holzforschung*, *77*(9), 700-712.

ii. Hartwig, M. & Gamstedt, E. K. (2020). On the composite design of wood branches leading to improved bending strength. In *IOP Conference Series: Materials Science and Engineering***,** 942(1), 012008.

Contents

1. Introduction

Without branches, trees would not become trees. They allow the tree to increase the surface exposed to sunlight for photosynthesis and accordingly formation of wood to heights not seen in herbaceous plants. Quantitively between 10 and 20% of the tree's total biomass are branches [1]. Still, branch wood and its formed reaction wood have so far been a less studied part of the tree. Reaction wood in conifers, i.e. compression and opposite wood, have been studied and summarised by Timell [2]. However, just a small potion of the studies were conducted on the compression wood (CW) found in the lower part of the branch and opposite wood (OW) found in the upper part of the branch. Since then very few studies have further looked into this research topic. A reason can be that traditionally it lacked applications in construction and furniture building compared to stem wood. There was no need, other than curiosity of nature's design, for expanding our knowledge on branch wood as a structural material, since it was mainly used as fuel in combustion. Gaining deeper insight in the the structure and behaviour of conifer tree branches can be beneficial both for a more sustainable forest and wood-based industry, as well as source of nature-inspired solutions for engineering problems.

1.1 Sustainability

Temperature increase, changes in precipitation patterns, increased wildfire risks due to climate change, together with increased damage by beetle attacks, result in a decline in European forest's biomass [3–5]. This means that less raw material for wood and wood-based products will be available, which will be detrimental for Sweden, where the forest industry contributes between 9 and 12% to the overall economy [6]. One solution to address this problem is the use of unused forest material. Or in other words, creating a need for raw forest materials that so far have been considered unsuitable and are mainly used as fuel. One of these raw materials is wood from branches and peaks of the trees. According to the Swedish Forest Agency, up to 80% of the branches and tree tops can and should be removed from the forest after felling. This raw product is one of the major sources of fuel from forest residues. It is predicted that this source will be getting bigger within the next 20 years; from 20-37 TWh to 30-39 TWh [7] .

So far, tree branches are an underutilized resource for wood and wood-based products on a larger scale, since hygromechanical properties as well as production processes differ immensely from stem wood-based products. By understanding this raw material better, the need of stem wood could be decreased by replacing it with branch wood. Furthermore, instead of using the branches only for fuel, but also in wood and wood-based products, leads to a more sustainable use of forest raw material, due to its further valorization.

Some first studies to characterise branch wood from decidious trees for future use in wood based products have been carried out [8, 9]. Olarescu et al. [9] has even produced and studied wood panel from branch wood of a limited number of conifer and decideous tree species.

The main focus in this work is on the branch wood of the two most common Scandinavian conifer tree species, Norway spruce (*Picea abies*) and Scots pine (*Pinus sylvestris*).

1.2 Biomimetics

Biomimetics is based on the idea to identify and understand principles in nature and to apply them to engineering problems. This makes it a multidisciplinary research field. Two strategies are commonly used in biomimetics; biology push and technology pull [10, 11]. Technology pull means that a problem is identified in engineering and a solution is looked for in nature. Biology push takes concepts from nature and applies the identified solutions in engineering. Hence, this approach gives a solution to an engineering problem, which was not identified before investigating the biological feature. The tree branch fulfilling multiple functions, like nutrient and water transport, as well as mechanical support offers a wide range of possible applications of solutions found within the hierarchical structure of the material. Wood has been of interest for biomimetics in multiple studies [12, 13]. The main focus has been to use the concept of fibre direction in form of the microfibril angle in wood to achieve desired mechanical performance. However, this only one of many adaptations that make the tree branch differ from stem wood. Could we gain even more by understanding the smaller levels of the hierarchy and gain new solution from abstracting them?

1.3 Aim and objectives

The aim of this thesis is gain deepen insight in the relationship between moisture variations and mechanical behaviour in branch wood, with the ultimate goal of contributing to the sustainable utilisation of wood material and transfering principles from the nature of branch wood on engineering problems. The objective of this thesis is to investigate the hygroelastic behaviour of branch wood by linking structural characteristics with hygroelastic properties at different length scales. Both experimental and modelling techniques, numerical as well as multiscale, are used.

In more detail, this is achieved by:

- Developing an analytical beam bending model to investigate bending resistance in softwood branches;
- Identifying swelling and elastic properties of CW and OW on micro level by compression testing and micro computed tomography
- Investing the swelling properties of CW and OW lignin by molecular dynamics simulation;
- Investigating the molecular structure of CW and OW lignin and microstructure of wood by synchrotron wide-angle X-ray scattering; and
- Investigating parameters than can affect swelling properties of the S2 cell wall layer in CW and OW by finite element modelling.

2. Conifer branch wood

Wood, a hierarchical biological material, has anisotropic material properties. Its unique structural features influence its properties. This enables an adaption of the branch wood to the mechanical loads connected to its position in the tree. First, the hierarchical structure and the differences between OW and CW at different levels are described. Thereafter, swelling and shrinkage behaviour due to moisture changes, as well as the mechanical properties are summarised.

2.1 Hierarchical structure

The hierarchical levels of wood as summarised by Gibson [14], Wohlert et al. [15] are presented in Figure 2.1 and explained in detail for CW and OW from the molecular level to the growth rings in the following section.

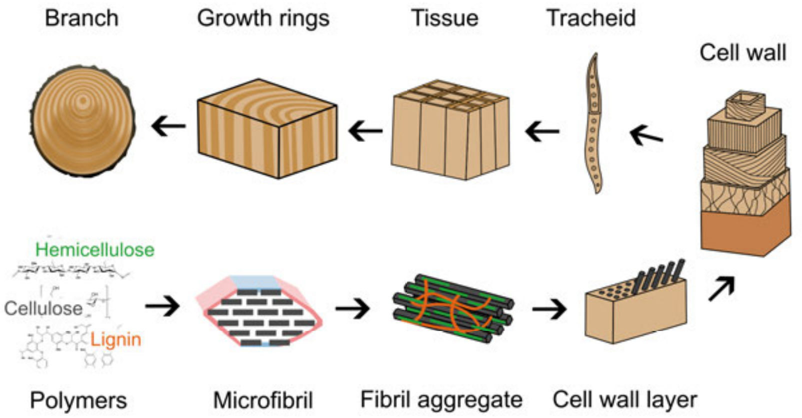

Figure 2.1. Hierarchical structure wood from the branch to wood polymers.

2.1.1 Microstructure

Individual wood polymers

The main components in all types of wood are cellulose, hemicellulose, lignin and extractives. These components differ chemically, as well as in quantity, for wood types found in conifer branches, namely CW and OW. In Table 2.1, their relative composition in Scots pine is summarised from literature [2, 16].

Table 2.1. *Chemical composition of stem wood and branch wood. The identified components are cellulose, hemicellulose, lignin and Other (like Ash, Resins & fats).*

	Cellulose (%)	Hemicellulose (%)	Lignin (%)	Other (%)	Literature
Stem wood					
	40.0	24.9	27.7	7.4	Ek et al. [16]
Branch wood					
CW	39.7-42.3	15.2-16.3	34.0-38.5	5.2-8.9	Timell [2]
OW	45.2-47.5	16.1-17.1	30.1-31.9	5.3-6.9	Timell [2]

Cellulose is a polysaccharide consisting of glucose units linked by $\beta(1 \rightarrow 4)$ linkages. Its biosynthesis is a process that occurs at the plasma membrane of plant cells. It forms a linear chain of 7000-15,000 units [14, 16]. In wood, the cellulose chains are forming slender fibrils of nanometer size in cross section, partially ordered in a crystalline form in so called cellulose microfibrils (CMFs) [17]. The CMs shape and number of chains is much debated lately. It was suggested that CMFs consist of 18-24 cellulose chains [18–20]. Even though often considered a crystalline material, its lattice is actually not defect free. Terrett et al. [21], Nishiyama et al. [22] have found disorders of the surface chains, as well as disorders periodically occurring along the length of the CMFs. There is no difference in intrinsic molecular structure between cellulose in CW and OW. However, less cellulose is found in CW [2].

Hemicellulose is a polysaccharide composed of different sugar units and linkages. Its biosynthesis is a process that occurs in the Golgi apparatus of plant cells. It is less linear than cellulose and consists of a backbone with side groups. In softwood, hemicelluloses are rich in mannose in the form of galactoglucomannan. Its backbone consists of mannose and glucose linked by $\beta(1 \rightarrow 4)$ linkages occasionally with side groups of galactose linked by $\alpha(1 \rightarrow 6)$ linkages to mannose [16]. In CW compared to NW and OW, significantly more galactose groups are present [2, 23, 24], making CW hemicelluloses more branched than OW hemicelluloses.

Lignin is an amorphous polyphenolic polymer. The monolignols are synthesized in the cytoplasm, and in contrast to cellulose and hemicelluloses the monomer units are transported to the cell wall where lignin is polymerised through random polymerisation [25]. Its exact structure and whether it is more branched or linear is under discussion [26]. Its variability due to the biosynthesis and its cross-linkages with hemicelluloses make it challenging to extract and analyse native lignin [27]. Softwood lignin consists mainly of cross-linked guaiacyl (G) lignin units. However, CW lignin contains also a significant amount of 4-hydroxyphenyl (H) lignin units. The monomers are linked by ether (C-O-C) and carbon-carbon (C-C) bonds. The ether bond β-O-4 is the most abundant bond in softwood. Common carbon-carbon bonds are β-5’ and 5-5’ [16]. Furthermore, more lignin is found in CW than OW and NW [2].

Water is always present in wood as cell wall water and/or capillary water, due to its hygroscopicity. Wood-water interactions are not solely causing swelling and shrinkage, but are equally important as the structure of wood for mechanical properties [28].

Fibril aggregates

In the plant cell wall, the microfibrils often form larger aggregated structures: fibril aggregates (FA, also called microfibrillar bundles or macrofibrils) [15, 17, 29]. When dried out, these aggregates are strongly bound together and resist both swelling and high levels of mechanical shear. Yet, microfibrils can be disintegrated from the FAs and individually dispersed in water[30]. It has been suggested that hemicelluloses may prevent aggregation by sorption to the microfibril surface so that hemicelluloses are trapped between the microfibrils [29]. While there is no comprehensive model available describing differences at FA level between CW and NW, the known differences in hemicellulose and lignin composition and distribution, likely result in differences at this scale.

Cell wall

Wood cells are hollow layered structures with a primary (P) cell wall on the outside and a secondary (S) cell wall and a lumen contained within. Between cells the middle lamellae (ML) are found. These parts fulfill different functions, where the P cell wall protects during growth, the S cell wall provides rigidity and the ML glues the cells together [31]. The S cell wall is divided into S1, S2 and S3-layer. The chemical composition and organization of CMF and the other components varies depending on the layer. Different layer also have different microfibril angle (MFA) [32, 33].

The ML is containing mostly lignin. In NW, the majority of the lignin is located in the ML, while in CW the ML is less lignified [34, 35]. The S cell wall of CW has a higher MFA than OW and NW. Usually in stem wood the MFA is around 0-5°. Branch wood has higher MFA with 30°reported for OW and 40°for CW [36]. The outer S2 layer of CW contains more lignin than in NW [34, 35] Furthermore, the S2 layer in CW is much thicker and tends to have helical fissures [37, 38]. CW lacks the S3 layer of the cell wall [37]. No differences between CW and OW have been reported for the P cell wall.

Tracheids

Tracheids account for 90-95% of the cells in wood. Tracheids are long hollow cells with a diameter of 14-46 μm and a length of 1.1-6 mm [16]. They assure both water and nutrient transport, as well as mechanical support. The tracheid cross-section of CW is more circular cross-section, while OW tracheids have a more hexagonal cross-section [2, 23, 39].

2.1.2 Macrostructure

Tissue

The lignins and pectins in the middle lamella connect the tracheids to a cell tissue. CW has intracellular spaces between the tracheids, due to the circular tracheid cross-section and a less lignified middle lamella.

Growth rings

Growth rings, consisting of earlywood and latewood are formed in the tree in annual cycle. Earlywood tracheids have a larger lumen, while latewood tracheids have a thicker cell wall. This leads to higher density in latewood. In CW, the growth rings are thicker than OW.

Branch

The branch cross-section is eccentric compared to stem wood, since the CW forms thicker annual rings. Furthermore, the higher lignin content in CW makes the CW appear darker in colour.

2.2 Elastic properties

The differences in the structure of OW and CW to adapt to its functions are reflected in the elastic properties of CW and OW in its unsaturated state. The comparison of experimental results is challenging, since results depend strongly on moisture content and experimental technique [40]. Furthermore, a major concern is the variation of elastic properties at the micro and macro level, due to the hierarchical structure of wood. Even within the macrolevel size effect are important to consider. This matters for modelling, since the size effect is not compatible with classical elasticity theory. It also means that comparing mechanical properties measured by different experiments can only be compared to a limited extent [41]. One such example is the modulus of elasticity (MOE) of Norway spruce at different scales. The MOE of the tracheids was determined as 17.4 GPa by Gindl et al. [42]. For latewood tracheids the modulus was 21.0 GPa and for earlywood tracheids 13.5 GPa [43]. Clear samples with growth rings had a much lower MOE with a value of around 7-10 GPa [44, 45].

The summarised elastic properties of branch wood and stem wood are just on macro scale, since these properties were not yet investigated at micro scale to our knowledge. For stem wood it is known that CW has a lower elastic modulus than stem wood , but elastic properties of branches have not been investigated extensively. The elastic modulus of branch wood, consisting of both OW and CW, compared to stem wood is lower. Timell [2] reported 10% lower stiffness for branch wood compared to stem wood of several American conifer species, as well as similar differences summarised for various conifer species. Scots pine branches even had a 75% lower MOE than NW with values of 3.32 GPa and 11.71 GPa respectively [46]. None of the studies determine the specific elastic properties of CW and OW in the tree branch. Furthermore, just stiffness in the longitudinal direction was measured.

The cellulosic microfibril are mainly contributing to the cell wall stiffness. Hence, the different MFA in branch wood compared to stem wood can explain the difference in elastic behaviour [36]. In addition, Bergander and Salmén [47] suggested based on simulations that also hemicellulose and lignin properties can affect the stiffness.

2.3 Moisture induced swelling and shrinkage properties

Wood, as a hygroscopic material, interacts with water throughout its lifetime. In its unsaturated state, changes in moisture lead to dimensional changes. Moisture desorption and absorption causes swelling and shrinkage.

In stem wood, the tangential swelling coefficient is two times larger than the radial, and 55 times larger than the longitudinal coefficient. Bengtsson [48] reports a tangential swelling coefficient of 0.33, radial swelling coefficient of 0.16, and a longitudinal swelling coefficient of 0.006.

Shrinkage of Norway spruce branches was reported by Timell [2]. In CW, the tangential shrinkage is more than two times higher than in OW, with values 3.1% and 7.8%. The radial shrinkage is similar to the tangential shrinkage for each wood type, with 3.7% shrinkage in CW and 8.8% in OW. Boutelje [49]found similar relation between radial and tangential shrinkage for Norway spruce and Scots pine at several locations in the tree branch. The longitudinal shrinkage is much higher in CW. In OW, the longitudinal shrinkage is 0.5%, while in CW it is 6.1% [2]. Volumetric shrinkage in CW is lower than in OW, with a range of 7.9–10.4% and 11.0–12.7% respectively.

The shrinkage is strongly affected by the different MFA in CW and OW, since the cellulose swelling is small. The larger MFA in CW facilitates longitudinal swelling and shrinkage and hampers the transverse changes, as has been studied for CW in the stem [50–53]. However, differences in MFA between OW and CW are lesser than between CW and normal wood in the stem [54]. This indicates that other structures contribute to the distinct swelling of OW and CW.

3. Multiscale approach

3.1 Multiscale experimental techniques

Non-destructive and in-situ experimental techniques have been beneficial for the investigations of hierarchical and hygroscopic biological materials, like wood [55]. Traditional techniques like light, electron and atomic force microscopy have given extensive insight in the microstructure of wood from the structure of cell wall layers to tissue level [56]. These techniques remain a valuable resource, but lack the possibility to investigate the effect of moisture and/or mechanical loading in real-time at the micro or macro material level and on smaller scale structures.

State-of-the-art techniques, like neutron and X-ray scattering, as well as X-ray computed tomography (XCT), allow in-situ testing of structures and the analysis of features at molecular, micro and macro level. XCT provides time-resolved 3D imaging (4D) of micro- or macrostructures by medical or micro XCT, respectively [57, 58]. Nowadays, it is a technique more commonly used for studying effects of moisture and/ or mechanical loading due to its 4D resolution. Furthermore, it allows to connect experimental with analytical methods through digital volume correlation to finite element modelling [59]. X-ray scattering techniques have been used in wood science mostly for studying properties related to the crystalline wood component, cellulose. Already in 1913, Nishikawa and Ono [60] reported the first fibre diffraction patterns of cellulose from wood. Scattering techniques complemented by solid-state nuclear magnetic resonance spectroscopy have given in the recent years new insight into the structure and interaction between wood polymers, as well as their interaction with water [20, 21, 61]. At the same time, modelling is an important component for interpreting results from techniques like X-ray scattering [62].

3.2 Multiscale modelling

Both for the fundamental understanding of wood and for providing useful predictions to engineers, developing models that capture the relationship between structural features and material properties is important. Because of the hierarchical structure of wood, modelling different levels separately without coupling can not capture the several mechanisms typically occurring simultaneously in wooden materials [63]. Theoretically, it is possible to model a wood

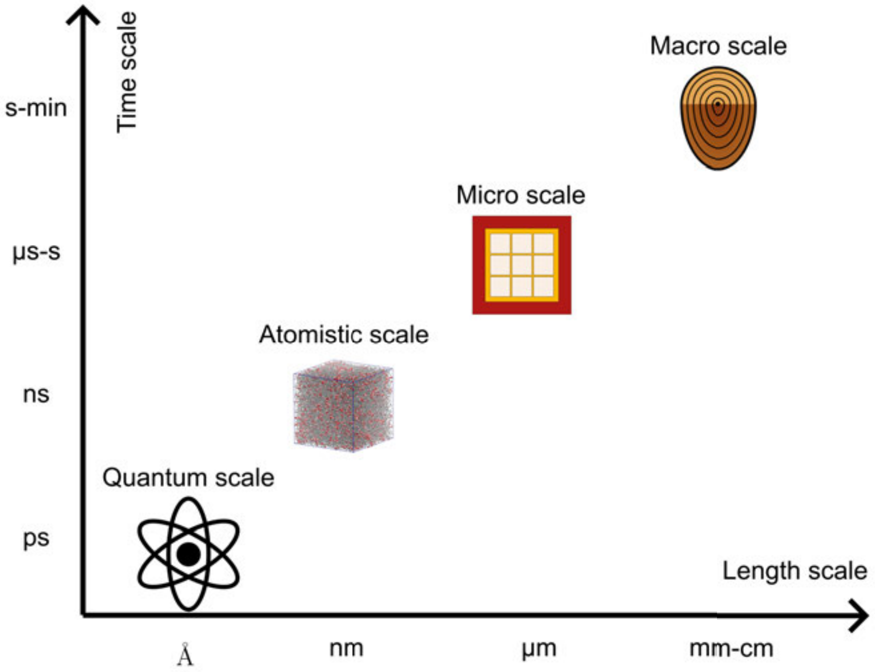

Figure 3.1. Scales in modelling of conifer branches.

with quantum mechanics or atomistic precision, but the long computational time and/or huge amount of computational resources needed makes it practically impossible. Hence, reality needs to be simplified in such a manner that continuum models can be applied. Multiscale modelling allows to simulate hierarchical materials and systems in a less expensive manner by reducing the need for computational power, or even make it feasible in the first place [64]. At the same time, it allows for a better accuracy than using just a larger scale modelling method. The scales and accordin time and length scales for modelling branch wood are shown in Figure 3.1.

In multiscale modelling for complex systems, two approaches are common:

- Coupling scales by using several models simultaneously, i.e *concurrent modelling*, and
- Coupling scales by information transfer from independent models, i.e *hierarchical multiscale modelling* [65].

Concurrent modelling is a common approach used for modelling cracks, material damage, free edges and interfaces. It is a suitable methods, where regions requiring a resolution at atomistic and molecular level, like the tip of the crack, while for other regions it is sufficient to be simulated as a continuum. These domains are coupled in the computational domain [65, 66]. This approach is useful for ordered crystalline materials, like metal, due to the limited spatial and temporal frame for its mechanism. However, it is less suitable for complex polymer composite materials, like wood, since phenomena occur simultaneously at different length scales and within levels at different time scales. Atomistic models capture only timescales of nano- to microseconds, which is for example not sufficient to simulate the water sorption in wood cell walls.

Hierarchical multiscale modelling has been used - amongst other things - for composite materials and wood. Information, relevant for a larger scale model, are determined with a smaller scale model, and passed on to the larger scale through information transfer [65]. Homogenisation of microstructures in wood as a form of hierarchical multiscale modelling has been studied in more detail during the last decades for a more efficient and accurate prediction of material behaviour on macro scale, e.g. Bengtsson [67]. Here, information can be transferred between continuum models [66]. Another relevant application of information transfer for wood material is the use of output from molecular dynamics simulations as the input for a finite element model [68]. Ciesielski et al. [63] suggests that coupling the MD or density functional theory (DFT) and continuum simulations is a promising approach to apply to a larger extent for modelling lignocellulosic biomass, but is currently understudied. Coupling molecular and continuum models is useful for understanding the effect of moisture on hygromechanical properties. This behaviour originates at the nanoscale, where water interacts with wood polymers, affects structures at larger scales, such as fibril aggregates, cell wall layers and cellular structure and finally at the tissue level, where swelling will be due to a combination of all these factors.

4. Results and analysis

In each paper that constitutes this thesis work, one or more hierarchical levels of wood structure and their relation to hygroelastic properties are investigated. A schematic illustration of the connection between each paper, methods used and the corresponding hierarchical level is shown in Figure 4.1. Firstly, studies at macroscopic and tissue level are presented in Paper I and II. Secondly, a closer look is taken at the molecular structure in Paper III and IV. Lastly, a connection between molecular and cell wall level is made in Paper V.

4.1 Paper I: Bending resistance of softwood branches

The aim of the first paper is to present an analytical model that demonstrates how tree branches are mechanically designed for elastic bending up to the limit state, considered as failure. This is achieved by considering an entire branch cross-section as a composite beam consisting of CW and OW. Material properties at macro level are taken into account to allow for a simple beam model.

The analytical model iss based on Euler-Bernoulli beam theory, hence, assuming the branch to be a slender beam and neglecting effects of shear. The relative amount of CW and OW is varied for an elliptical composite beam cross-section to study the effect of CW content on bending resistance. Elastic modulus and limits for elastic behaviour are input parameters used to determine a maximum bending moment for different CW content. In addition, the location within the branch is predicted to reach elastic limit first.

Previous experimental characterisation has shown CW content in branches to be between 25 and 50%. Interestingly, this coincides with the maximum allowed bending moment that is found to have an optimum for CW content between 35 and 75%. The analysis of stress distribution show that up to 35% CW content, compressive stresses in OW govern the stress profile, while above 35%, tensile stresses in OW will be most critical.

Despite its simplicity, this model is able to predict the mechanical optimisation for bending in tree branches. A suggestion and comparison for bio-inspired engineering and classical engineering solutions for composites was provided.

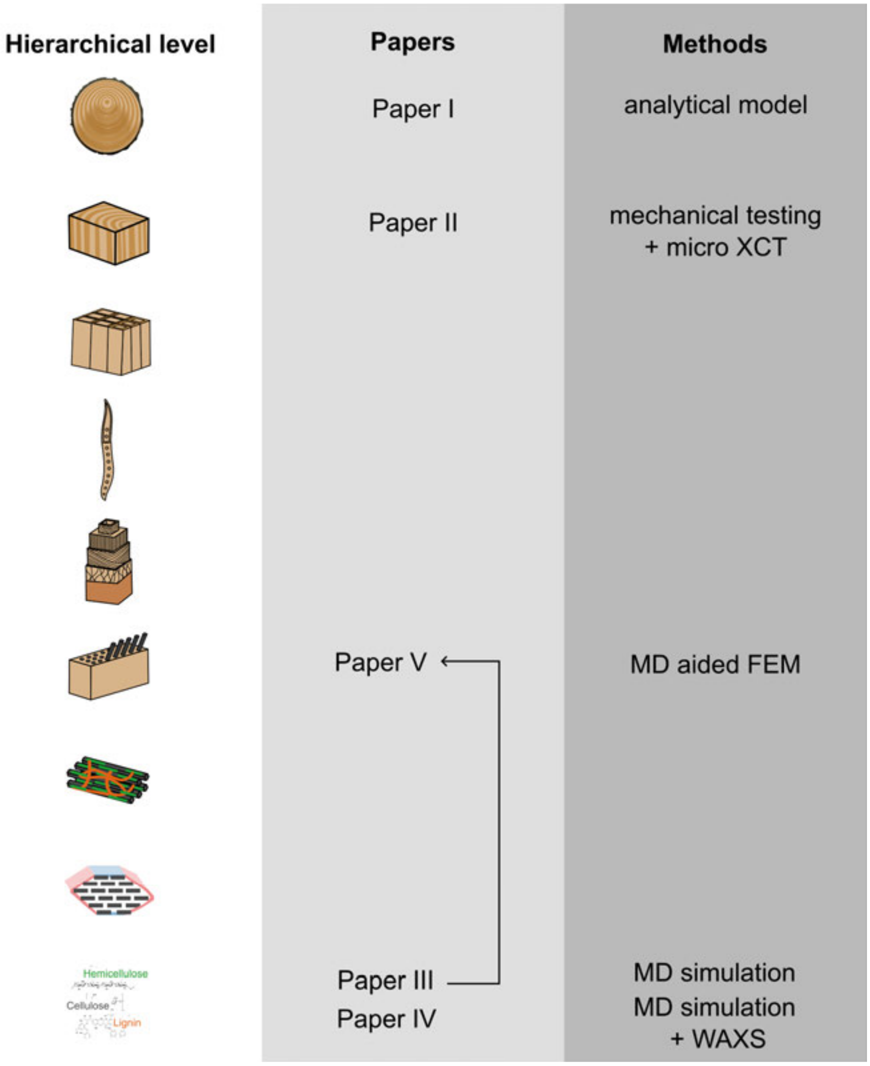

Figure 4.1. Illustration of structural features and properties studied in the different papers and the respective methodology.

4.2 Paper II: Hygroelastic properties of compression and opposite wood

The study presented in the second paper focusses on closing the knowledge gap of branch wood material properties. Swelling and elastic properties of CW and OW at the macrostructural level are investigated by 3D tomographic imaging and mechanical characterisation in longitudinal and two transverse directions.

Specimens of CW and OW are conditioned at different levels of relative humidity. Swelling is observed by lab-based micro XCT imaging and subsequent image analysis, while the elastic modulus is obtained through compression testing. Material properties like MC and density are reported. Additionally, the MFA is determined by synchrotron wide-angle X-ray scattering.

CW is found to have a longitudinal swelling coefficient 11-12 times larger than OW, while the transverse swelling coefficient is just half of the coefficient of OW. Swelling behaviour in CW seems to be less anisotropic than in NW. The elastic moduli of CW and OW is lower than the modulus of NW. For CW, the longitudinal elastic modulus is lower than for OW, but it decreases less with increased moisture content. The density has no significant effect on the hygroelastic properties. The MFA is around 43°and 51°for OW and CW, respectively. The difference in MFA contribute to the differential swelling and elastic behaviour of CW and OW.

Questions on the origin of these different swelling properties of CW and OW arise: Which structural features contribute to the swelling properties? Could the different chemical composition of lignin in OW and CW play a role?

4.3 Paper III: Swelling behaviour of compression and opposite wood lignin

In the third paper, a molecular modelling study is presented that builds on simple models of CW and OW lignin to investigate the swelling properties of both materials by MD simulations. The starting point is to look at the possible effect of different chemical structures of CW and OW lignin on the swelling properties of both CW and OW departing from the knowledge gained in Paper II.

The models are built according to the fact that CW lignin has a higher frequency of 4-hydroxyphenyl (H) lignin units compared to OW wood, that is assumed to be built of cross-linked guaiacyl (G) lignin units only. Lignin tetramers of four G-units (GGGG) or three G-units and one H-unit (GGGH) linked by β-O-4' linkages, are chosen to represent OW and CW and simulated in systems with 1000 tetramers and varying moisture content under constant pressure and temperature.

Differences in swelling, structure and water dynamics are found, even though the OW and CW tetramers only differed by one lignin unit. CW lignin is found to have a slightly, but significantly, higher uniaxial swelling coefficient than OW lignin. This is attributed to the distribution of water. The phase separation between lignin and water is more pronounced for CW lignin compared to OW. This behaviour is linked to structural differences, where intermolecular $\pi-\pi$ stacking is more common in CW lignin and hydrogen bonding to water more pronounced in OW lignin.

While this study recognises a small but significant difference in structural response to increased water content and swelling coefficient of CW and OW lignin, it can not lead to any conclusions on the effect of this difference on the swelling properties of CW and OW tissue. However, the differentiation in molecular swelling is an important piece of information to transfer into models at larger scale.

4.4 Paper IV: Structural analysis of compression and opposite wood lignin

The focus in the fourth paper is on further analysing structural features of lignin of CW and OW and its interaction with water at molecular level. WAXS measurements are performed on lignin from CW and OW. The results are compared with MD simulations based on Paper III.

A mild organosolvent extraction of lignin allows to obtain structurally-intact lignin from CW and OW. The lignin powder is conditioned at three different levels of relative humidity for WAXS measurements to analyse the effect of moisture on CW and OW lignin structure. The T-shaped and sandwich π-π stackings of the aromatic rings in lignin were determined from the scattering plots. Furthermore, the MD model systems GGGG and GGGH described in Paper III are used to determine π-π stackings, as well as to obtain scattering pattern by the Debye equation. These results are complemented by NMR spectroscopy to gain insight in functional groups and linkages prevalent in the different types of lignin.

WAXS measurements showed that the distance of sandwich π-π stacking is similar for CW and OW lignin with a value of around 3.8 Å. CW lignin has a longer distance for the T-shaped π-π stacking than OW lignin with distances of around 5.1 Åand 4.7 Å, respectively. CW contained 22 to 30% T-shaped π-π stackings and 70 to 78% sandwich π-π stackings, while OW contained nearly equal amounts of sandwich and T-shaped π-π stackings. It stands out that CW lignin distances and content of π-π stacking interactions are dependent on relative humidity, but not the same is found for OW lignin.

Distances and content determined by MD simulations are compared to the experimentally obtained values. Distances of T-shaped and sandwich stacking from MD are slightly higher than the experimentally obtained distances, and there is no difference seen between OW and CW lignin. The content of sandwich and T-shaped π-π stacking interactions is dependent on the lignin type. CW lignin contained more H-units than OW lignin, while it contained less β-0-4 linkages.

The simulations of CW and OW capture the structural features, particularly π-π stackings, analysed by WAXS to some extent. Discrepancies between experiments and simulations can be due to: the simplification of lignin to tetramers and the use of only one type of linkage in the simulations; MD simulations not being as suitable for studying π-π stacking as density functional theory; and challenges in analysing scattering data of amorphous materials.

4.5 Paper V: Swelling behaviour of cell wall of compression and opposite wood

The aim of the final study is to demonstrate a hierarchical multiscale modelling. Hierarchical in the sense that it starts with MD simulations results of lignin, and together with the estimated properties of the other constituents predicts cell-wall swelling where the ultrastructural arrangement of the biopolymers are considered. The difference in swelling of the S2 cell wall of CW and OW is investigated by FE modelling integrating the minor but significant difference in swelling coefficients of CW and OW lignin obtained in Paper III to evaluate whether the difference actually would impact the cell walls swelling behaviour. MFA of CW and OW obtained in Paper II are included.

A representative volume element of the cell wall subjected to variation in moisture content is modelled by FE methods. Therefore, transversely isotropic cellulose microfibrils are embedded in isotropic hemicellulose and lignin. Periodic boundary conditions allowing free swelling are applied. Recent data from experiments and MD simulations are used as input for material properties. Three parametric studies are performed to understand their effect on the cell wall swelling coefficient. These parameters are the lignin content, swelling coefficient of lignin and the MFA.

The MFA affects the swelling coefficient the most, while lignin content and the swelling coefficient the least. However, higher lignin content and swelling coefficient contribute both to higher transverse swelling. The obtained swelling coefficients are of the same magnitude as swelling coefficients obtained by experiments on tracheids, as well as tissue.

The different structure of CW and OW lignin seems to have no major impact on the swelling properties of the cell wall. The investigated parameters, more specifically the variation in MFA, can partly explain the different swelling coefficients in CW an OW. It clearly indicates, that structures, which are not considered in this study, both at larger hierarchical levels, as well as at same or smaller levels are influencing the swelling coefficient.

5. Conclusions

Branch wood is an understudied wood material, differing from stem wood at multiple hierarchical levels, but has the potential to contribute to a more sustainable use of forest resources, as well as serving as an inspiration in biomimetics.

In this thesis hygroelastic properties of conifer branches, and more precisely the specific properties of CW and OW, were investigated.

First, the branch is analytically modelled as a bi-material composite beam of CW and OW. The study confirms that the presence of OW and CW in branches leads to mechanical optimisation towards bending. The model is clearly limited by the lack of data for elastic properties of CW and OW. Hence, for allegedly the first time these properties were measured for CW and OW of branches. Especially, the swelling behaviour of CW and OW is different which gave rise to questions about how structural differences at separate length scales affect uniaxial swelling at tissue level. Therefore, in the subsequent work, focus was shifted from analysing the macrostructure to investigating the nano- and microstructure and its effect on swelling of CW and OW tissue.

The second part of the thesis moves down to the nanostructure and focuses especially on the differential swelling properties linked to the structure of CW and OW lignin by wide-angle X-ray scattering supported by MD simulations to clarify their contribution to the differential swelling of CW and OW. The swelling coefficient of CW lignin was higher than the coefficient of OW lignin due to the different phase separation of water and lignin. While the molecular scale experiments and simulation could provide detailed insights into structural preferences of CW/OW lignin and their response to changes in moisture, such isolated lignin behaviour is not necessarily identical to the role of lignin swelling inside the cell wall in CW/OW tissue. Therefore, the thesis work is concluded by demonstrating an approach where molecular and cell wall level modelling is combined, studying the effect of differential swelling of CW and OW lignin on a fraction of the cell wall using the material properties from MD simulations in a FE model. Complementary parameters, like lignin content and MFA, are also considered. The hierarchical multiscale modelling shows that the differences observed in differential swelling of CW and OW tissue are barely influenced by the variation in swelling properties of CW and OW lignin. However, the different structure of CW and OW lignin can instead affect the mechanical properties and accordingly the hygroelastic properties of CW and OW itself.

Overall, the thesis is not just giving insight into wood-moisture interactions of branch wood, but also into multiscale experimental and modelling techniques relevant for understanding hygroelastic behaviour of wood in general. The effort trying to obtain a holistic picture of wood swelling at multiple length scales shows that there are several mechanisms (e.g. variation in MFA and lignin swelling) acting simultaneously, and that only a multiscale approach will be able to capture its driving forces.

In-situ micro-CT and X-ray scattering are invaluable resources for analysing both structure and behaviour of wood under mechanical loading and controlled climate. Challenges remain though in data analysis and interpretation for both X-ray techniques. Hierarchical multiscale modelling by coupling MD simulations and FE modelling via information transfer shows to be a useful tool to gain knowledge on moisture related behaviour of wood. However, determining suitable parameters to be simulated by MD for the information transfer can be challenging.

Being a small step toward a full description of wood hygromecanics, this thesis is far from covering all aspects of structural and related hygromechanical properties of CW ad OW in the branch. The thesis is a starting point that has given rise to several ideas for useful future investigations, both from a scientific and engineering perspective. Selected potential future research topics in the field hygroelastic properties of branch wood are suggested below:

- Hierarchical multiscale modelling is a valuable method for connecting different hierarchical levels in wood. This has been used to a limited extent for transferring information between molecular and continuum level in wood science. Apart from lignin swelling coefficients, this approach can contribute to obtaining and using elastic properties of lignin. In addition, variation in hemicellulose and its role in hygroelastic properties can be investigated.
- Structural analysis of lignin by X-ray scattering give new insight into lignin chemistry. Due to its chemical variability and being an amorphous solid, analysis of scattering data remain a challenge. This research area would benefit from testing a lignin-based material with simple and known structure to compare with MD simulations and/or Density function theory.
- Lastly, it would be exciting to take the next step to a more efficient use of forest resources by manufacturing and testing a branch wood based product. For example, developing a chipboards, that uses the less anisotropic swelling properties of CW to its advantage.

Svensk sammanfattning

Trä är ett förnybart konstruktionsmaterial som använts allt sedan förhistorisk tid. På senare år har trä kommit att användas alltmer i konstruktioner som alternativ till armerad betong och stål. Likaså kan trä fungera som råvara för att ersätta förpackningsmaterial av plast från olja. Denna utveckling drivs framför allt att trä utgör ett hållbarare alternativ och i slutändan leder till minskat koldioxidutsläpp jämfört med konventionella material.

I skogsbruk vill man använda så stor andel av träden som möjligt till förädlade produkter. Efter fällning är det svårast att använda grenar och trädkronor till byggmaterial eller biomassa. Det beror i huvudsak på att deras form och struktur skiljer sig åt mot den mer homogena stammen. Grenarna innehåller en annorlunda vävnad, kallad reaktionsved, som hjälper dem att bära last samt att kontrollera position och tillväxt. I barrved kallas denna reaktionsved för tryckved eftersom den befinner sig på grenens trycksida, dvs undre sida. Veden på den övre dragbelastade sidan av grenarna är mer lik den normala veden som finns i trädets stam.

För att utnyttja hela trädet bättre, inklusive dess grenar, som råmaterial för vidare förädling så behövs mer kunskap om tryckvedens struktur och egenskaper. Trä har en hierarkisk struktur, alltifrån den molekylära skala, i cellväggarna, i själva cellerna, längs årsringarna, olika typer av ved och upp till trädet i sin helhet. Egenskaper på en större global längdskala berör på struktur och lokala egenskaper i alla underliggande längdskalor i den hierarkiska strukturen. Andra tillverkade konstruktionsmaterial har som regel inte denna hierarkiska design. Syftet med detta avhandlingsarbete är att studera struktur och egenskaper hos tryckved i flera längdskalor, både experimentellt med beräkningsmodeller. Det är en förhoppning att denna nya förståelse kan på lång sikt vara av nytta för att bättre ta till vara på grenmaterial innehållandes tryckved. En annan aspekt är att trä har optimerats för att bära last och transportera näring under miljontals år, och att det möjligtvis kan finnas uppslag på smarta konstruktionslösningar genom att studera träets struktur och lastbärande mekanismer. Denna disciplin kallas biomimetik. Många konventionella material är isotropa och homogena, dvs. de är lika starka överallt och i alla riktningar. En bättre resurshushållning vore att göra materialet starkt och orienterat just där det behövs. Trä är ett exempel på ett sådant smart material. I kompositmaterial med starka fibrer inbäddade i ett lastöverförande matrismaterial försöker man åstadkomma liknande effekter som finns hos trä, men man har inte kommit på när lika långt som i träets optimerade hierarkiska struktur.

Om vi börjar i den minsta skalan, den molekylära, så har beteendet hos en av träets polymerer - ligninet - i cellväggen studerats både med molekylärdynamiska simuleringar och med Röntgen-spridning. Ligninet har olika kemisk struktur i tryckved jämfört med övrig ved. Vidare är ligninet en restprodukt från massatillverkning, vilket skulle kunna användas till framställning av biobaserade plaster i större grad än vad som nu är fallet, då lignin ofta bränns för att alstra värme och energi. Simuleringarna visade att fuktsvällningen skiljer sig något mellan lignin från tryckved med den från övrig ved. Röntgen-mätningarna visade sig stödja uppskattningar från simuleringarna.

I en finit-element-simulering på cellväggsnivå visade sig fuktsvällning bero i största grad på hur cellulosafibrillerna är orienterade och mindre utsträckning på andel och typ av lignin som finns i cellväggen. Det är känt att tryckved har en större vinkel mellan cellulosafibrillerna och cellernas riktning, vilket bidrar till tryckvedens större fuktsvällning i träfibrernas riktning jämfört med veden från övriga delar av grenarna. Detta har konstaterats med fuktsvällningsmätningar i datortomograf-experiment.

På grennivå så har en enkel balkmodell utvecklats och använts med indata för styvhet och styrka för de olika vedtyperna i drag och tryck. Det visade sig att avvägd andel av tryckved gav största kapacitet för böjmoment, vilket också återspeglas i den faktiska fördelningen av tryckved i ett grentvärsnitt.

Det finns många tänkbara möjligheter för fortsatta studier av både vetenskapligt och ingenjörsmässigt intresse. En är att studera ligninet från tryckved och hur det kan användas för vidare förädling. En annan är att bättre försöka förstå hur grenar är konstruerade för att bära last på ett optimerat sätt och ändra riktning vid tillväxt, för att sedan utnyttja denna kunskap i tillverkning av kompositmaterial. En annan är att använda bestämma de hygroelastiska egenskaper hos grenar och kvistar för att förutsäga deformationer i timmer när trä torkas och återfuktas. Detta skulle möjliggöra bättre utnyttjande av trämaterial innehållandes ved från grenar.

Acknowledgments

First, I would like to express my gratitude to my supervisors. Kristofer Gamstedt, thank you for giving me the opportunity to freely develop this research project. It was challenging and exciting at the same. I would not have been able to reach so far without your support, Malin Wohlert and Sara Florisson. Your insight in a variety of methodologies and your vast knowledge on wood has been a great inspiration to me. I am very glad you are equally intrigued by branch wood as I am. Thank you all three for the encouragement and invaluable discussions. It has been a pleasure working with you. I would like to thank Carolin Öhman for the support in technical and theoretical issues related to the micro CT.

My studies have been enriched by a number of collaborations. I am immensely grateful to Alexandr Nasedkin for your major contribution by modelling lignin. Emiliano De Santis and Nil Tabudlong Jonasson, thank you for joining this work. I am thankful to all collaborators at KTH: Martin Lawoko, Maria Karlsson and Fika Andriani. Thank you, Tomas Rosen, for your patience and willingness to share your knowledge.

I would like to thank all my former and current colleagues of the division of Applied Mechanics for a pleasant atmosphere and for providing a glimpse in a variety of research topics within mechanics.

I am thankful to my fellow Ph.D. students for sharing insightful discussions, as well as wonderful memories. Danial, Klara and Anna, you always managed to brighten the day up a bit more and I am glad that a friendship developed out of our common journey.

Finally, I would like to thank my family for both your practical and emotional support along this journey. Your understanding and endless patience has made all the difference.

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Acta Universitatis Upsaliensis

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Editor: The Dean of the Faculty of Science and Technology

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2024