Wood-water interactions investigated with simulated and experimental scattering

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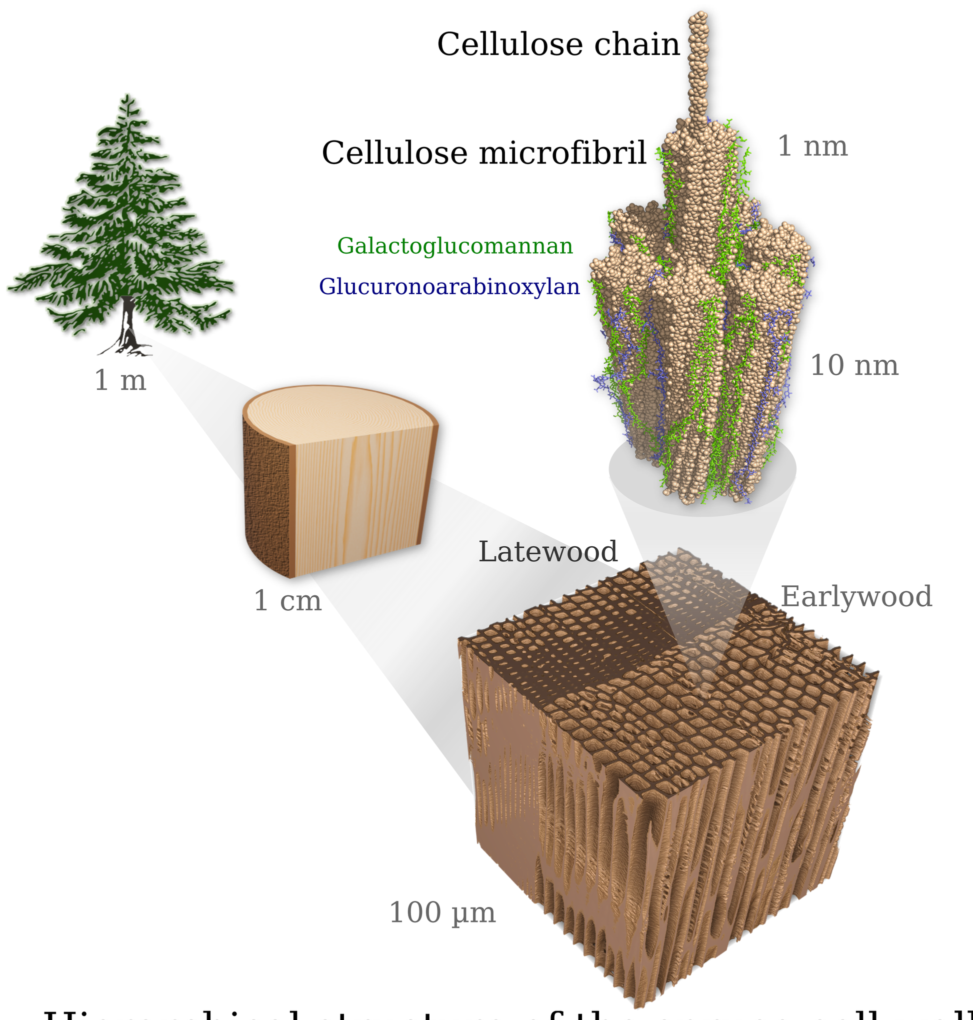
1. Introduction

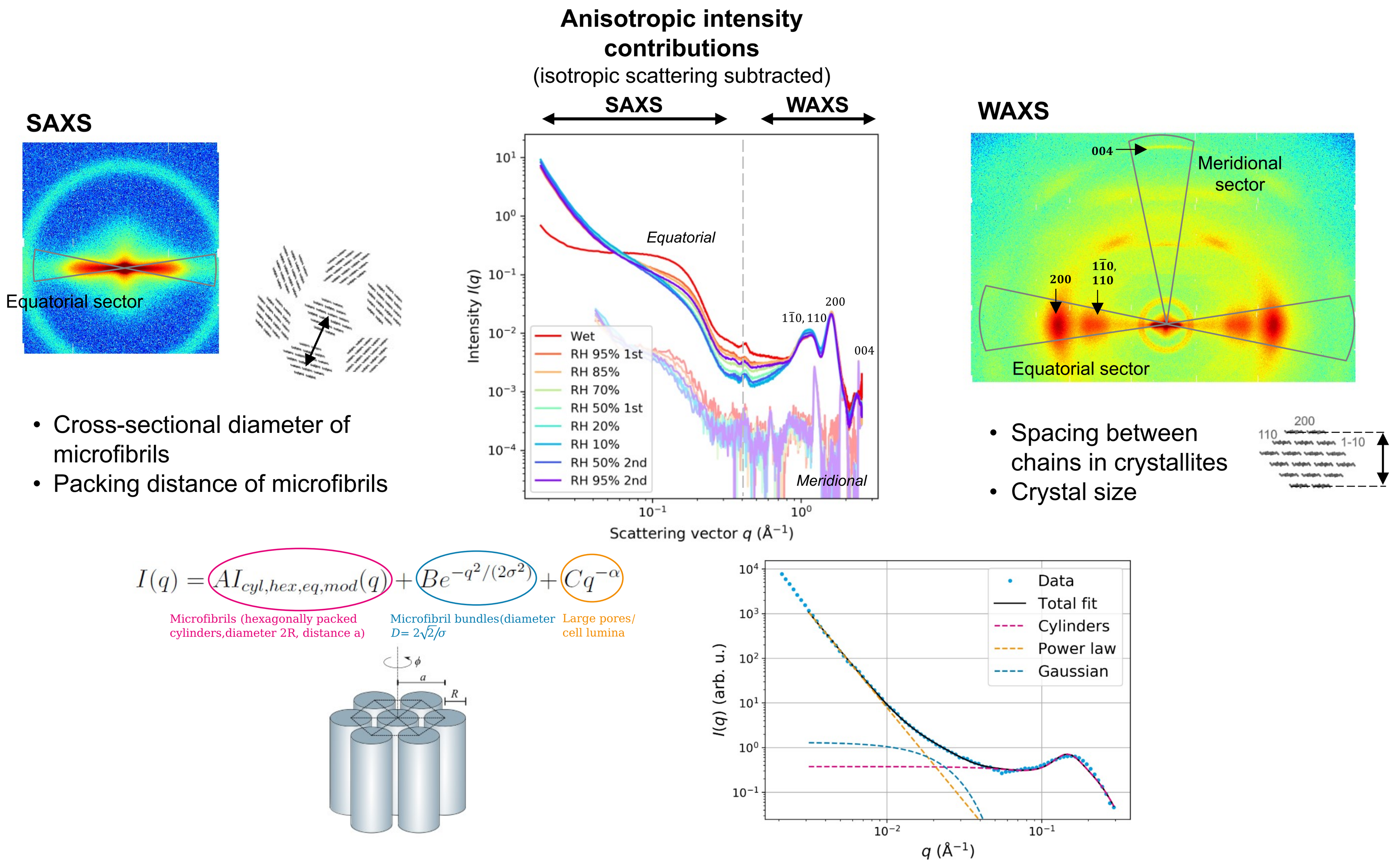
The macroscopic properties of wood derive from the microscopic structure of the plant cell walls and depend greatly on the moisture content. However, measuring in-situ changes in wood nanostucture due to moisture is challenging. Scattering measurements allow for non-destructive characterization of changes inside wood cell walls.
Combining both molecular dynamics simulations and tailored scattering measurements [1,2,3] provides complementary results about the nanostructure and moisture behavior of wood. Comparing simulated scattering data with experimental results sheds new light into the wood nanostructure and how it responds to moisture [4].



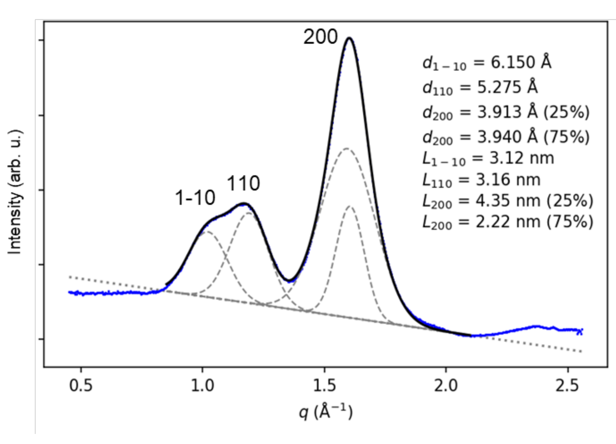
Hierarchical structure of the spruce cell wall

2. Scattering investigates the nanostructure

Scattering at different angles probes the structure at different length scales. Small-angle X-ray scattering (SAXS) provides insight into the size and packing of microfibrils, while wide-angle X-ray scattering (WAXS) gives information about the crystalline lattice of individual fibrils.



The above model [2] based on closely packed infinite cylinders can be fitted to equatorial small-angle scattering contribution from wood.

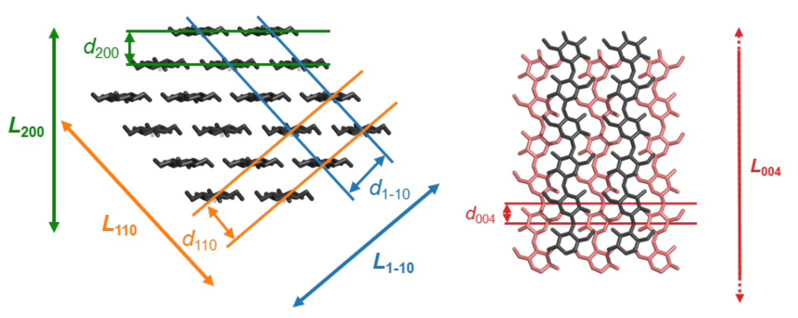


Bragg law:

$$d_{hkl} = 2\pi / q_{hkl}$$

Scherrer equation:

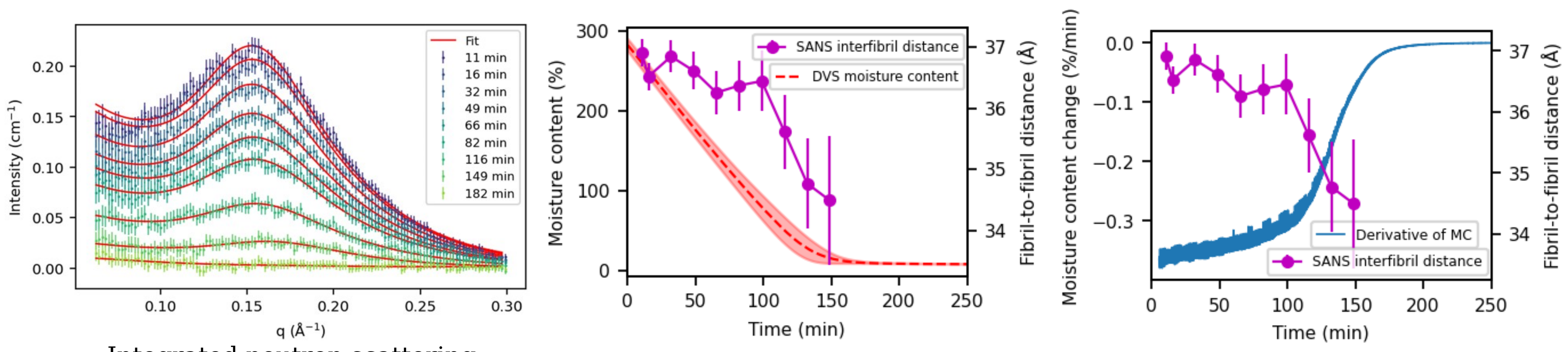
$$L_{hkl} = \frac{2\pi}{\Delta q_{hkl}}$$



Wide-angle scattering peaks and the corresponding crystal lattice directions. Peak location corresponds to d-spacing of the crystal, while peak width has an inverse correlation with crystal size.

3. Moisture response experiments

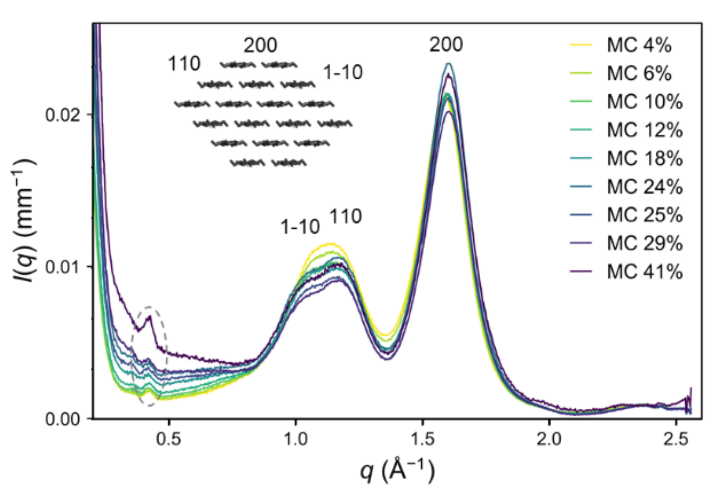
Small-angle neutron scattering (SANS) experiment of drying wood reveals how microfibril bundle deswelling corresponds with a change in drying behavior from a constant drying rate to falling rate [1]



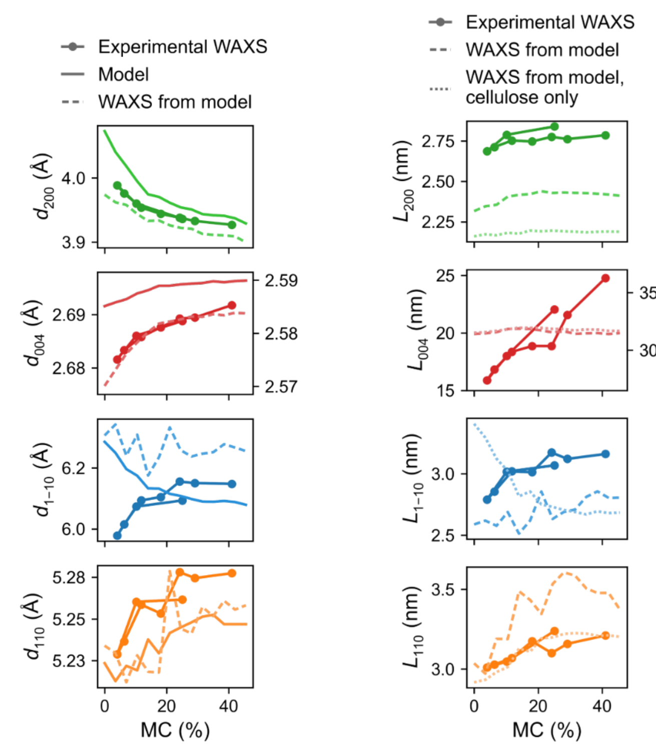
Integrated neutron scattering

Interfibril distance compared with moisture content and its change

X-ray scattering experiment in controlled humidity tracks structural changes at different moisture equilibriums.



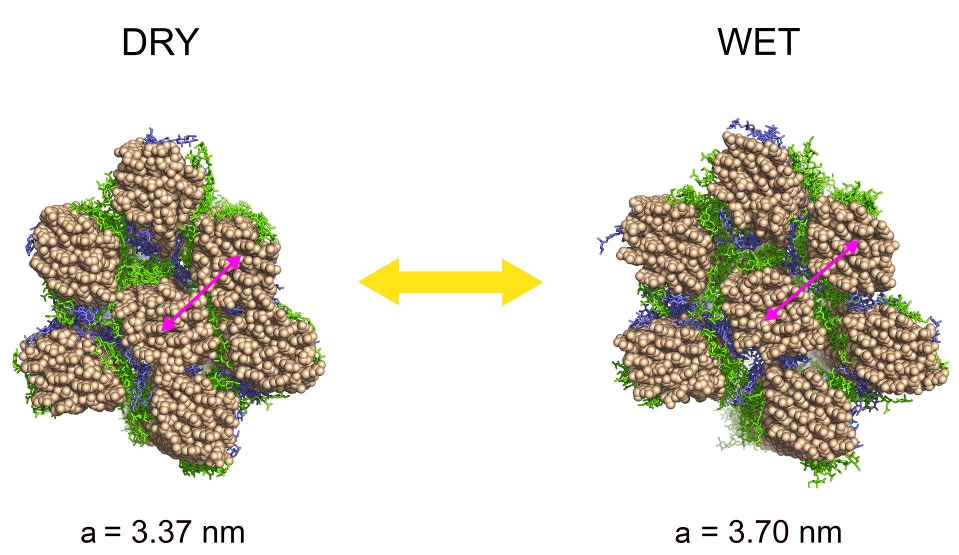
Integrated X-ray scattering at different moisture contents



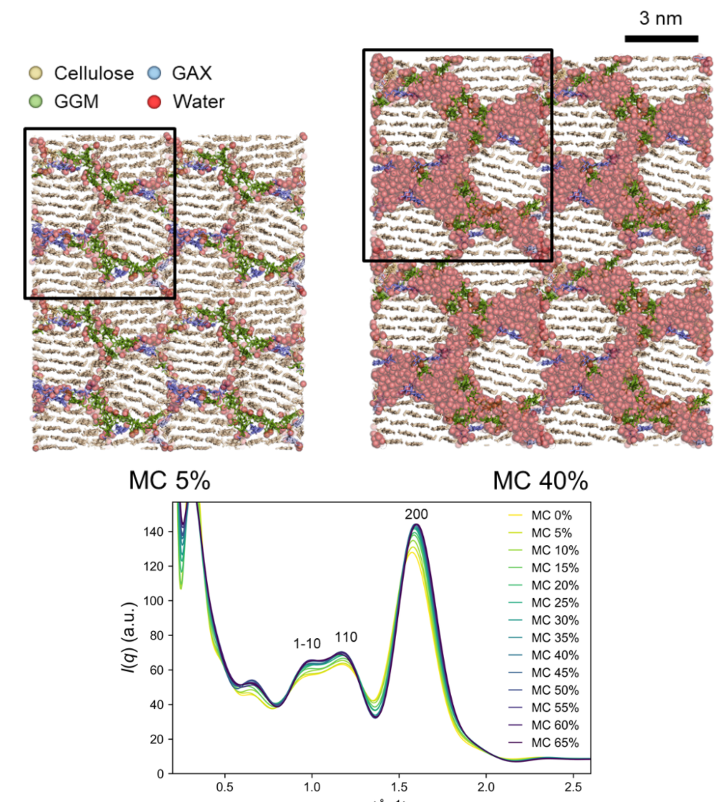
Fibril d-spacing (d) and crystal size (L). Experiments compared with simulations

4. Combining experiments with simulations

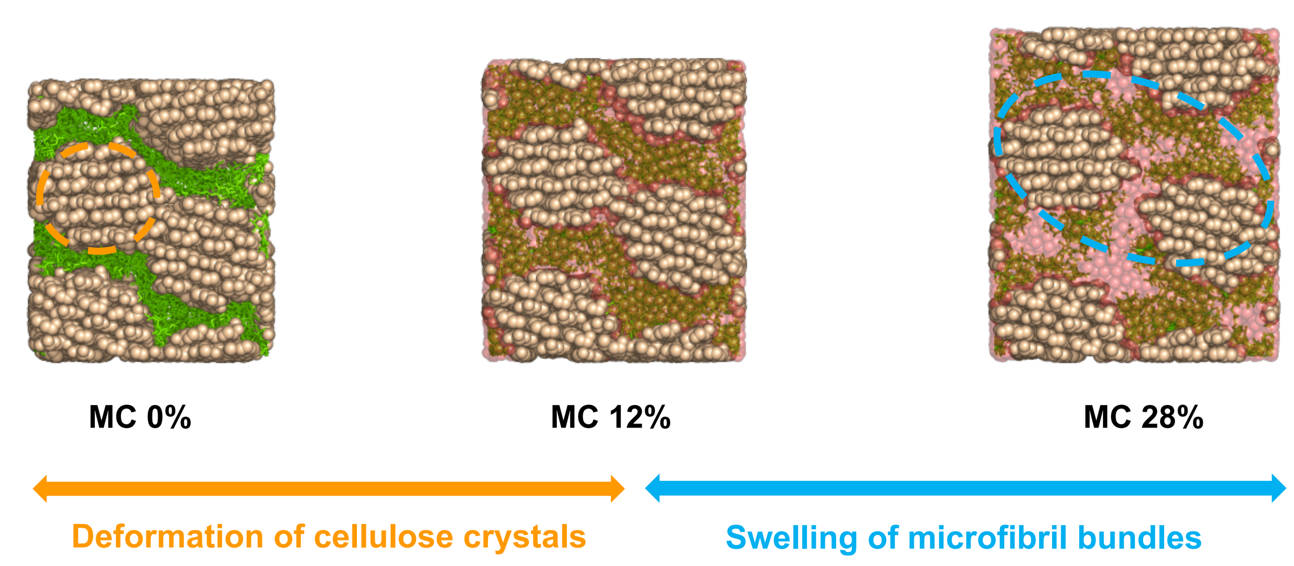
Microfibrils along with hemicelluloses on their surface are simulated using Molecular Dynamics. The scattering from the resulting structures can be then mathematically calculated. The results will then be compared with measurements.



Microfibril bundle model shows similar moisture response to neutron scattering



Simulted periodic microfibril lattice produces similar scattering and moisture behavior as X-ray experiments



Our work demonstrates different drying regimes. Changes in the crystal lattice occur at low moisture content (MC), while changes in fibril packing occur at higher MC. At even higher MC (above fiber saturation point), packing changes are diminished due to saturated cell walls, as seen in neutron scattering results.

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References

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