Contribution ID: **605** Type: **Poster (+) Presentation**

Hygromechanical mechanisms of wood cell wall revealed by molecular modeling and mixture rule analysis: Role of components, interphases and hydrogen bonding

Wednesday, 2 June 2021 16:00 (1 hour)

Wood is a natural porous bio-polymeric material with complex hierarchical structure. Owing to its exceptional mechanics and sustainability, wood has been an essential material for mankind, in both conventional applications, e.g. building material, and future advanced systems, e.g. green electronics. Sorption of environmental moisture strongly affect wood mechanics, due to the intrinsic nanoscale porosity and hydrophilicity of wood cell wall material. Despite the numerous studies on wood mechanics, fundamental mechanical aspects of moisture-induced phenomena such as swelling, weakening, shape memory effect, etc, remain to be fully elucidated in view of wood hierarchical structure.

For investigating the wood cell wall nanostructure and the physical nature of wood-water relationship, this study presents a state-of-the-art atomistic model of softwood cell wall layer, taking great care to reflect the state of knowledge of wood molecular structure. Individual polymer components, their mixtures, composites and interfaces are mechanically characterized in separate simulations, gathering an unprecedented micromechanical dataset including hydrogen bonding, swelling and weakening, over the full hydration range. Quantitative agreement with available experimental reports is achieved. Based on the rich dataset, material models based on mixture rule uncover the impact of intermolecular interactions and identify the role of different components and their interactions with water. The most critical factors determining wood mechanics on the nanometer scale, and in particular the pivotal role of interphases, indicating an interaction between different polymeric components, are highlighted. Especially, it is shown that the hemicellulose glucomannan plays the role of a glue between the reinforcing crystalline cellulose and other matrix components, showing a moisture-sensitive anisotropic interphase zone. The work gives thought to the origin of wood cell wall orthotropy, moisture-induced weakening and swelling, each a different manifestation of the strong coupling between the mechanical and hygric behavior of wood.

Time Block Preference

Time Block A (09:00-12:00 CET)

References

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Primary authors: Dr ZHANG, Chi (ETH zurich); Prof. KETEN, Sinan (Northwestern University); Dr COASNE, Benoit (CNRS/University Grenoble Alpes); Prof. DEROME, Dominique (Universite de Sherbrooke); Prof. CARMELIET, Jan (ETHZ)

Presenter: Dr ZHANG, Chi (ETH zurich)

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