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Molecular Mechanisms Underlying The Treatment of Archaeological Wood Cell Wall Composite with Polyethylene Glycol: A Hybrid Monte Carlo and Molecular Dynamics Study

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Treatment of wood cell wall with polyethylene glycol (PEG) is a widely used technique by archaeologists and conservators to consolidate waterlogged archaeological wooden artifacts such as the Swedish warship Vasa and Henry VIII's warship the Mary Rose. During the decade-long consolidation process of introducing PEG solution into these wooden artifacts, PEG molecules gradually diffuse into the wood cell wall and replace the water molecules. PEG treatment is found to stabilize the wood structure and prevent extreme shrinkage and structural collapse during the following slow drying process altering the hygromechanical properties of wood in response. Due to the chemical complexity and hierarchical intricacy of the wood structure, PEG-cell wall interactions are governed by various entangled multi-scale mechanisms which are yet to be elucidated and distinguished.

This work attempts to provide a molecular-level understanding of the impact of PEG treatment on the hygromechanical properties of wood-cell wall components, including amorphous cellulose, hemicellulose (galactoglucomannan), uncondensed lignin (coniferyl and sinapyl) and fiber-matrix interphase. To this aim, an iterative hybrid all-atom molecular dynamics and grand canonical Monte-Carlo (GCMC) simulation is employed to examine the hygromechanical properties of polymeric mixtures, including sorption isotherm and sorption hysteresis and sorption-induced swelling. The structure of mixtures of biopolymers and PEG equilibrated under a range of relative humidity from fully dry to saturation is then characterized by measuring porosity, pore size distribution, mechanical properties, and hydrogen bonding network.

The amorphous cellulose mixtures treated with PEG show reduced moisture adsorption and swelling at museological conditions (40-60% RH), followed by an unfavorable increased sorption/swelling at high relative humidity, highlighting a crossover phenomenon in hygroscopicity. In comparison, lignin mixtures show less substantial moisture/swelling reduction indicating that PEG treatment is more effective on polysaccharide polymers of wood. The cellulose nanocomposite model reveals the concentration of PEG at the fiber-matrix interface, which disturbs the fiber-matrix hydrogen bonding network and consequently enhances the moisture sorption and mechanical softening at the interface. Comparing the simulation results with predictions from an enhanced rule of the mixture model reveals the key role of interphase and synergic interaction between PEG and wood polymers. The enhanced mixture model enables us to characterize two molecular mechanisms governing the consolidation at the nanoscale. First, the filling of existing nano-sized pores in the amorphous structure by PEG as relatively small PEG molecules fill the vacancies previously available for the adsorption of water molecules. Second, the network of wood polymers confines PEG polymers and prohibits PEG from further swelling, thus reducing its water sorption. This behaviour of PEG may be a characteristic to look for when considering novel consolidant materials in the future.

Participation

In-Person

References

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Primary author: SHOMALI, Ali (ETH Zurich)

Co-authors: Dr ZHANG, Chi (ETH zurich); Dr LIU, Wenqiang (Sherbrooke University); Dr COASNE, Benoit (CNRS/University Grenoble Alpes); Prof. J. SCHOFIELD, Eleanor (The Mary Rose Trust); Prof. DEROME, Dominique (Universite de Sherbrooke); CARMELIET, Jan (ETHZ)

Presenter: SHOMALI, Ali (ETH Zurich)

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