MOLECULAR MECHANISMS INVOLVED IN TREATMENT OF WATERLOGGED ARCHAEOLOGICAL WOOD WITH POLYETHYLENE GLYCOL: A HYBRID MONTE CARLO AND MOLECULAR DYNAMICS STUDY

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Treatment of wood cell wall with polyethylene glycol (PEG) mixtures impregnation has been proven a successful technique for consolidation of waterlogged archaeological wood during the drying process and stabilizing its hygromechanical response. Although widely used in practice, due to the complex hierarchical structure of wood and molecular scale nature of consolidation with PEG, various mechanisms proposed to explain the interaction between PEG polymers and wood cell wall are yet to be elucidated. In this study, an iterative hybrid all-atom molecular dynamics and grand canonical Monte-Carlo (GCMC) simulation [1] is employed to prepare mixtures of amorphous cellulose and uncondensed lignin with PEG200, hydrated in a range relative humidity from fully dry to saturation pressure. The sorption isotherms and swelling curves are then provided to investigate the hygroscopic properties introduced by PEG treatment. The treated samples show reduced moisture adsorption and sorption-induced swelling at museological conditions. The equilibrated mixtures structure is then characterized by measuring porosity, pore size distribution, mechanical properties, and hydrogen bonding network. Comparing the simulation results with predictions from the rule of mixture reveals the key role of interphase and synergic interaction between PEG and wood polymers in elevated stability of PEG-treated samples, which can be attributed to two molecular mechanisms. First, the filling of nano-sized pores in the amorphous structure as relatively small PEG molecules fill the vacancies previously available for the adsorption of water molecules. Second, the confinement of PEG polymers in the solid frame of wood polymers prohibits PEG from further swelling and reduces its water sorption. These properties of PEG may be a characteristic to look for when considering novel consolidant materials in the future.

REFERENCES

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