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The Effect of Water Molecules on Mechanical Properties of Cell Walls NIMA RAHBAR, SINA YOUSSEFIAN, Worcester Polytechnic Institute — The unique properties of bamboo fibers come from their natural composite structures that comprise mainly cellulose nanofibrils in a matrix of intertwined hemicellulose and lignin called lignin-carbohydrate complex (LCC). Here, we have utilized atomistic simulations to investigate the mechanical properties and mechanisms of interactions between these materials, in the presence of water molecules. The role of hemicellulose found to be enhancing the mechanical properties and lignin found to be providing the strength of bamboo fibers. The abundance of Hbonds in hemicellulose chains is responsible for improving the mechanical behavior of LCC. The strong van der Waals forces between lignin molecules and cellulose nanofibrils are responsible for higher adhesion energy between LCC/cellulose nanofibrils. We also found out that the amorphous regions of cellulose nanofibrils is the weakest interface in bamboo Microfibrils. In presence of water, the elastic modulus of lignin increases at low water content and decreases in higher water content, whereas the hemicellulose elastic modulus constantly decreases. The variations of Radial Distribution Function and Free Fractional Volume of these materials with water suggest that water molecules enhance the mechanical properties of lignin by filling voids in the system and creating Hbond bridges between polymer chains. For hemicellulose, however, the effect is always regressive due to the destructive effect of water molecules on the Hbond of its dense structure.

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