Neutrons and Simulation Reveal Coupling of Dynamical and Mechanical Properties of Cellulose

Objective:

- Understand how hydration influences cellulose mechanics and dynamics.

Approach:

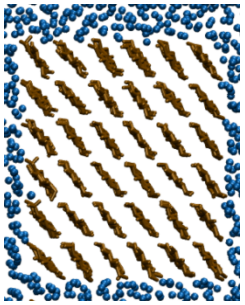
- Molecular dynamics simulations and dynamic neutron scattering experiments probed the structure and nano-second dynamics of cellulose fibers at different temperatures and degrees of hydration.

Results:

- Hydrated cellulose exhibit higher fluctuations than dry samples. Surface hydroxymethyl atoms determined the experimental hydration dependence.
- 20% hydrated cellulose is more rigid than dry cellulose fibers. (We note that most field-dried biomass wood or grass has 20% moisture.)
- Increase in conformational disorder of the surface with temperature follows the cellulose rigidity (persistence length). This implies coupling between structural and mechanical properties of cellulose.
- Paper accepted for publication in *Biomacromolecules*.

Significance:

- Detailed description of how hydration-dependent fluctuations and disorder at the cellulose surface lead to enhancement of cellulose fiber rigidity. This supports the importance of moisture in biomass structure and strength.



cellulose hydration

hydroxymethyl disorder

fiber rigidity

Part of the BER Biofuels SFA at ORNL

Petridis, L.; O'Neill, H. M.; Johnsen, M.; Fan, B.; Schulz, R.; Mamontov, E.; Maranas, J. K.; Langan, P.; Smith, J. C., Hydration Control of the Mechanical and Dynamical Properties of Cellulose. *Biomacromolecules* **2014**, DOI: 10.1021/bm5011849.

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