Neutron and X-Ray Experiments and Computational Modeling of Pretreatment of Biomass

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Project Goals:
Lignocellulosic biomass comprises the vast majority of biomass on Earth and has the potential to play a major role in generation of renewable biofuels if cost-effective conversion can be achieved. Largely composed of plant cell walls, it is a complex biological composite material that is recalcitrant to the structural deconstruction and enzymatic hydrolysis into sugars that is necessary for fermentation to bioethanol. The Scientific Focus Area in Biofuels is developing “Dynamic Visualization of Lignocellulose Degradation by Integration of Neutron Scattering Imaging and Computer Simulation” for multiple-length scale, real-time imaging of biomass during pretreatment and enzymatic hydrolysis. This is providing fundamental information about the structure and deconstruction of plant cell walls that is needed to drive improvements in the conversion of renewable lignocellulosic biomass to biofuels.

Abstract
Lignocellulosic biomass is potentially an important non-edible renewable organic source of energy and chemical feedstock. However, biomass is difficult to exploit in practice because it resists degradation to glucose in industrial hydrolysis processes and thus requires expensive thermochemical pretreatments. Understanding the mechanism of breakdown of the hydrated matrix of hemicellulose and lignin polymers that encrusts the glucose-rich fibrous cellulose during these thermochemical pretreatments will lead to more efficient use of biomass. However, characterizing the morphology of biomass as it evolves in response to thermochemical pretreatment has been difficult because of its hierarchical structure and the complexity of its components. By combining multiple probes of structure, sensitive to different length scales, with molecular dynamics simulations, we reveal some fundamental processes responsible for the morphological changes in biomass during steam explosion pretreatment. We further show that the basic driving forces are the same in some other leading thermochemical pretreatments, such as dilute acid pretreatment. The compensation between the entropy and enthalpy of hydration drives the cell wall components over kinetic barriers, destabilizing them, and causing irreversible morphological changes. Our findings suggest that new pretreatments and plant modifications that promote lignin and hemicellulose phase separation and increase the porosity of the cell wall matrix while preventing increases in cellulose crystallization as a result of dehydration will improve biomass conversion.