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Plant cell wall structural studies during thermochemical deconstruction using neutron scattering

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The Center for Structural Molecular Biology (CSMB) at Oak Ridge National Laboratory (ORNL) is a national user facility funded to support and develop the user access and science research program of the Biological Small-Angle Neutron Scattering (Bio-SANS) instrument at the High Flux Isotope Reactor (HFIR). Bio-SANS is dedicated to the analysis of the structure, function and dynamics of complex biological systems. The CSMB also operates a Bio-Deuteration Laboratory located at the Spallation Neutron Source (SNS) for deuterium labeling of biological macromolecules in support of the biology neutron scattering program. This resource complements capabilities at other Department of Energy (DOE) Office of Biological and Environmental Research (OBER) facilities for structural biology, and also supports studies of biomass recalcitrance and biomembranes as part of the DOE Genomic Science Program. In-situ small-angle neutron scattering (SANS) and molecular dynamics (MD) computer simulation were used in a combined approach to examine real-time breakdown of biomass through acidic, basic and ionic liquid thermochemical reactions. Cellulose, a major carbohydrate in biomass is understood to undergo significant change, between crystalline and non-crystalline states. Most enzymes optimally hydrolyze amorphous cellulose to ethanol than crystalline cellulose. Consequently, thermochemical reactions have been targeted to disrupt the crystalline state of cellulose. Here, we report real-time SANS experiments during dilute acid and alkali pretreatment of poplar using a bulky reaction cell. Dilute acid, like most acidic pretreatments exhibit an increase in the crystallite dimensions of the cellulose microfibril. While alkali pretreatment does not show a change in the cellulose microfibril dimension even though during the treatment significant shrinking and swelling in the cellulose microfibril was observed. Overall, these results highlight the evolution of cellulose microfibril structure when subjected to different thermochemical reactions.

Primary authors: Dr PINGALI, Sai Venkatesh (Oak Ridge National Laboratory); Dr O'NEILL, Hugh (Oak Ridge National Laboratory); Dr DAVISON, Brian (Oak Ridge National Laboratory)

Presenter: Dr PINGALI, Sai Venkatesh (Oak Ridge National Laboratory)

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