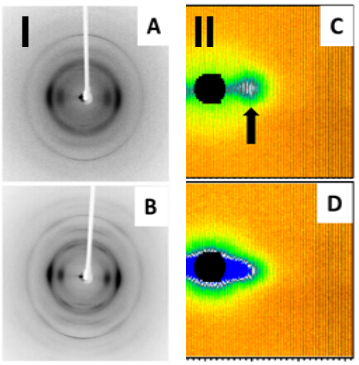
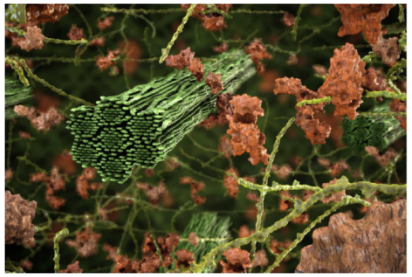
Neutrons Probe Common Processes Responsible for Structural Changes during Biomass Pretreatment



(I) Wide-angle x-ray fiber diffraction and (II) small-angle neutron fiber diffraction patterns collected from *P. tremuloides* chips (biomass) that were untreated (A and C) and SEP-treated (B and D). X-ray diffraction spots became sharper after SEP, indicating increased cellulose crystalline size, and an equatorial neutron diffraction feature (indicated by black arrow in C) suggested a structural side-by-side packing of cellulose fibrils.



Visualization of lignin aggregation on cellulose fibers based on high-performance computer simulations provided comprehensive understanding.

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Scientific Achievement

Neutron scattering, in conjunction with x-ray diffraction and molecular dynamics simulation, revealed fundamental processes responsible for morphological changes in biomass during steam explosion pretreatment (SEP). The unique capability of contrast variation using neutrons—a technique of varying the scattering power of an element to investigate structure—was critical to determining these structural changes.

Significance and Impact

Understanding biomass structural changes during pretreatment could lead to new pretreatments and plant modifications that promote lignin and hemicellulose phase separation, increase porosity of the cell wall matrix, and prevent further cellulose crystallization. All offer advantages to the biofuel industry by accelerating and improving biomass-to-ethanol conversion.

Research Details

- Key processes responsible for structural changes are cellulose dehydration and lignin-hemicellulose phase separation.
- Basic processes are the same in some other leading thermochemical pretreatments, such as dilute acid pretreatment.

P. Langan, L. Petridis, H. M. O'Neill, S. V. Pingali, M. Foston, Y. Nishiyama, R. Schulz, B. Lindner, B. L. Hanson, S. Harton, W. T. Heller, V. Urban, B. R. Evans, S. Gnanakaran, A. J. Ragauskas, J. C. Smith, B. H. Davison. *Green Chemistry* 16 (2014): 63–68.

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