NREL Highlights SCIENCE

# Cellulose Simulations Demystify High-Temperature Behavior

Molecular simulations that model cellulose microfibrils at high temperature indicate regions that may be easier to break down, which could lead to more efficient processing of cellulose into biofuel.

Using molecular dynamics simulation, scientists at the National Renewable Energy Laboratory (NREL) have modeled cellulose microfibrils at 230°C to learn how temperature affects the nanoscale structure of cell wall components of plants.

In plants, individual microfibrils that comprise cell walls are twisted rods—3.5 nanometers thick—made of chains packed together in rope-like structures thousands of nanometers long.

Heat is an essential tool in the process of breaking down plants to produce liquid fuels. Many changes occur in the cell wall due to heating, but these changes have not been well understood at the molecular level and are difficult to study experimentally.

Through molecular simulations, NREL scientists have shown that heating causes sections of the microfibrils to be straightened. The "twist" in the microfibrils is compressed into very short regions that may be easier to break down than the crystalline straight sections.

Experimentally, deconstruction rates of heat-treated cellulose are significantly faster at the beginning of hydrolysis than at the end. We hypothesize that the highly twisted regions are more susceptible to hydrolysis and therefore break down first, with the straighter regions remaining resistant—consistent with the experimentally observed leveling off in rate.

Another discovery from simulations is that the pattern of hydrogen bonds allows protons to be transferred through the crystal lattice in a preferred direction. This insight helps us to understand the material properties of cellulose and, in particular, the hydrogen bonding network that is responsible for its high stability.

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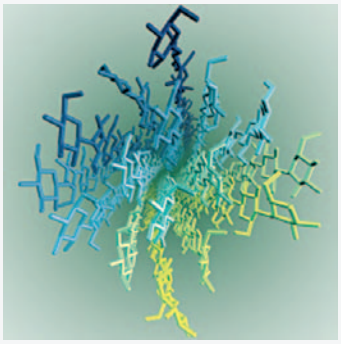
**References:** J.F. Matthews, M. Bergenstrahle, G.T. Beckham, M.E. Himmel, M.R. Nimlos, J.W. Brady, and M.F. Crowley (2011), "High-Temperature Behavior of Cellulose I," *J Phys Chem B* **115**(10), 2155–2166. doi: 10.1021/jp1106839



## Key Research Results

### Achievement

NREL scientists used molecular dynamics simulation to model cellulose microfibrils at 230°C to learn how temperature affects the nanoscale structure of plant cell wall components.

### Key Result

Heating causes sections of microfibrils to straighten, concentrating twist in very short regions. Also, hydrogen bond patterns allow protons to move through the cellulose lattice in a preferred direction.

### Potential Impact

This new understanding of cellulose behavior at high temperature may lead to a better understanding of the hydrolysis process and a more efficient means of breaking down cellulose.

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