Center for Lignocellulose Structure and Formation

CLSF

U.S. DEPARTMENT OF ENERGY

an Office of Basic Energy Sciences
Energy Frontier Research Center

PENNSTATE 1855 · NC STATE UNIVERSITY · Virginia Tech 1872

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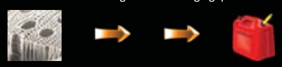
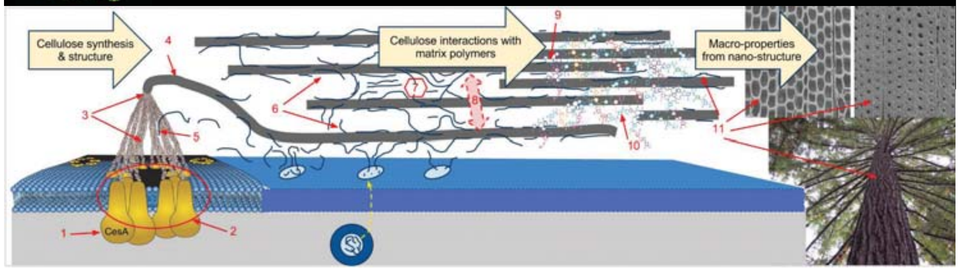
Much of the energy captured by photosynthesis is locked up in plant cell walls in a form called **lignocellulose**. If lignocellulose (or 'cellulosic biomass') could be economically converted into a liquid biofuel, it could help replace petroleum. However, lignocellulose is recalcitrant to biochemical conversion due to its complex and poorly-understood structure. Filling this knowledge gap is the focus of CLSF.





CLSF Research topics (diagrammed above):

1. Cellulose synthase (CESA): structure and mechanism of β-1,4-glucan polymerization.
2. Cellulose synthesis complex (CSC): protein composition and operation to produce a cellulose fibril.
3. Cellulose crystallization: biophysics and energetics.
4. Cellulose fibrils: native structure and bundling; interaction with water, enzymes.
5. Entrapment of xyloglucan, other matrix polymers in nascent cellulose microfibril; consequent changes in cellulose structure and wall network formation.
6. Binding of matrix polysaccharides to cellulose surfaces; mechanisms of binding, binding energies, adhesive forces; binding geometries; competition among polymers for binding surfaces.
7. Cross-linking of adjacent cellulose microfibrils to one another; direct binding; cross linking of matrix polysaccharides with other matrix polymers.
8. Microfibril and matrix polymer movements during cell wall extension and surface expansion.
9. Bundling of cellulose microfibrils into large structures; nature of bundling, changes in fibrillar structures.
10. Lignification: interaction of lignin with cellulose surfaces & matrix polysaccharides; cross linking of lignin to wall polysaccharides and proteins; wall rigidification & dehydration.
11. Multi-scale modeling of cell wall structure to account for cell wall porosity, water flows, mechanical properties, enzymate accessibility & degradation.

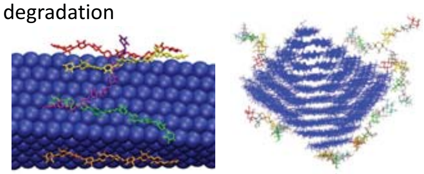
Cell wall architecture and dynamics

Visualizing cellulose fibril networks and changes after physical perturbation yields new insights into cell wall dynamics

Atomic force micrograph of cell wall. Image credit: T. Zhang.

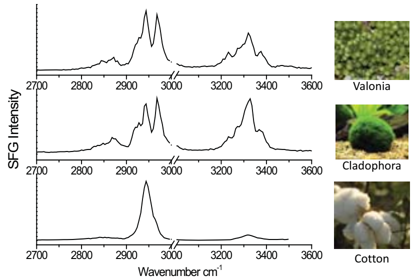
Cellulose structure and its interactions with matrix polymers

Computational modeling can clarify fundamental mechanics of cell wall cohesiveness and recalcitrance to enzymatic degradation



Computational models of a cellulose fibril with matrix polymers bound to its surface. Surface view (left) and cross-section (right). A cellulose fibril is a semi-crystalline array of ß-1,4 glucan polymers (blue) that interacts with matrix polymers such as xylan (various colors) on its surfaces. Image credits: L. Zhong and Z. Zhao.

Spectroscopy analyzes variations in cellulose structure within cell walls



Natural cellulose varies in structure; SFG (sum frequency generation vibration) spectroscopy has been newly shown to distinguish structural features of cellulose from different biological sources. Image credit: S. Kim.

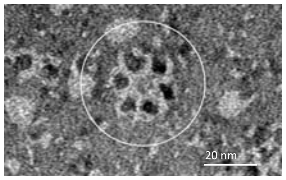
Major Research Questions

(1) How does the cellulose synthase complex produce cellulose microfibrils?
(2) What are the physicochemical interactions among cell wall components that lead to a strong network and what are the steps in their assembly?
(3) How do macro-scale properties of cell walls (mechanics, porosity, thermal properties, etc.) emerge from nano-scale properties of cell wall components?

All of these questions are being attacked by multi-investigator and multi-approach techniques.

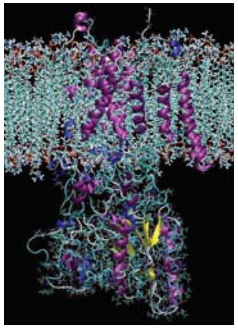
Probing the structure and function of the cellulose synthesis machinery

A multi-protein cellulose synthase complex (CSC) within the plasma membrane produces cellulose fibrils



Electron micrograph of a rosette-type CSC (circled) within the plasma membrane of a plant cell. Rosettes contain numerous cellulose synthase enzymes that produce the glucans that make up a microbril. Image credit: C. Haigler.

Cellulose synthase (CESA) – a key protein within the CSC



Putative molecular model of a single CESA associated with the plasma membrane. CESA has not yet been crystallized but new *ab initio* computational protein folding reveals the approximate 3D CESA structure, which in turn clarifies how it functions. Image credit: Y. Yingling.

CLSF Mission

To elucidate the nm-scale structure of bio-polymer networks in plant cell walls and their means of assembly, to provide a basis for improved conversion of biomass into fuels and improved biomaterials.

Network structure and properties

Genetic and enzymatic experiments determine how matrix components contribute to cell wall properties

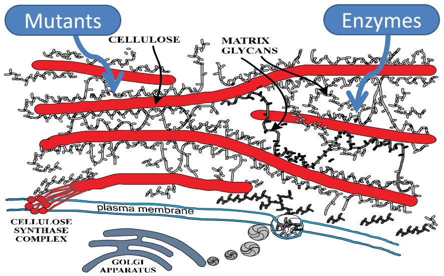
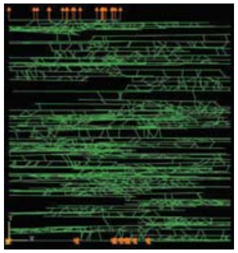


Diagram illustrating experimental approaches. Mutants deficient in specific wall matrix components are analyzed for changes in cellulose crystallinity and fibril bundling, cell wall extensibility, and related characteristics. In addition, specific enzymes are used to remove single components, followed by assays of cell wall properties with spectroscopic and mechanical methods. Image credit: D.J. Cosgrove.

Computational modeling of cell walls explores how macroscale properties (e.g. Young's modulus) depend on nanoscale cell wall properties



Properties of cellulose fibrils and matrix polymers (green lines) were incorporated into a finite element model of cell wall mechanics. Physical strains (orange arrows) are applied, and the resulting stresses are calculated. Image credit: V. Puri and H. Yi.