The Shape of Native Plant Cellulose Microfibrils

Scientific Achievement

Determined the preferred arrangements of cellulose chains in microfibrils as formed in plant cell walls.

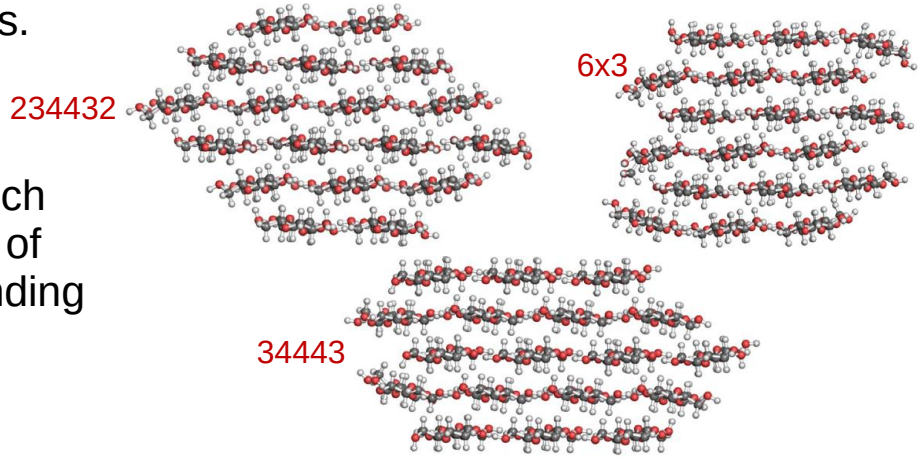
Significance and Impact

Cellulose microfibrils form the scaffold upon which plant cell wall architecture is based. Knowledge of the shape of the fibril enables deeper understanding of matrix polymer interactions with microfibril surfaces and for modeling microfibril formation.

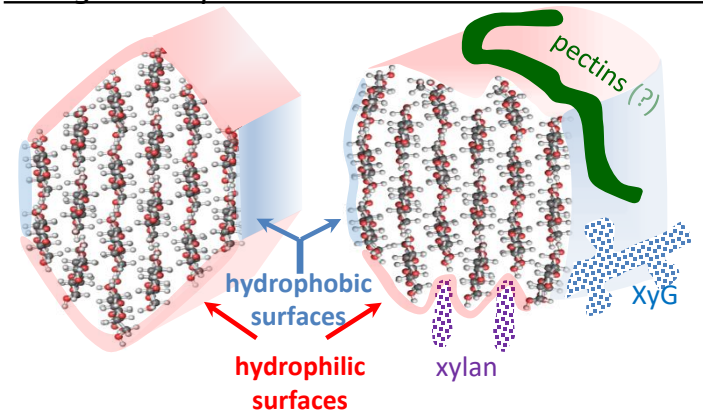
Research Details

- Three potential shapes made up on 18 chains were tested. They differ in hydrophilic and hydrophobic surface areas and conformations.
- Quantum mechanical calculations were compared to experimental data to determine which model best reproduces experimental observations.
- A novel arrangement of five layers in a 3-4-4-4-3 shape was preferred.

Possible arrangements of cellulose microfibrils based on 18 cellulose chains



Background: potential cellulose-matrix interactions



Work was carried out at UTEP, PSU and ORNL. Kubicki JD, Yang H, Sawada D., O'Neill H, Oehme D, Cosgrove D (2018) The shape of native plant cellulose microfibrils, *Scientific Reports 8:13983. DOI:10.1038/s41598-018-32211-w*