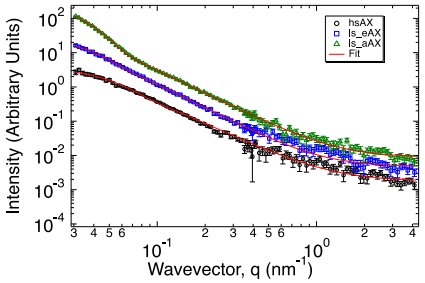
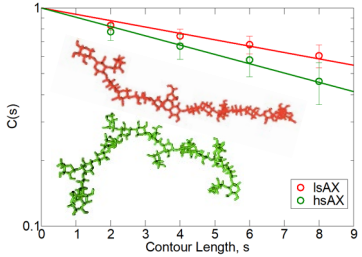
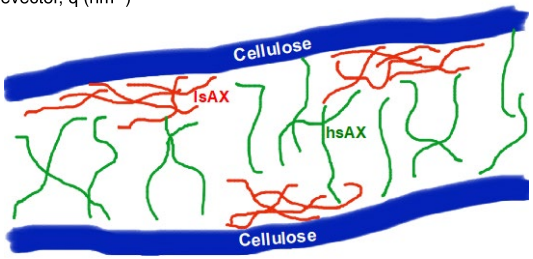
Effect of Arabinose Side-Chain on Xylan Rigidity and Self-Aggregation







Top left: SANS data shows low substituted arabinoxylan (lsAX) aggregates more than its high-substituted (hsAX) counter part. **Top right:** Tangential correlation function showing hsAX is more flexible than lsAX. **Bottom**: Hypothetical arrangement of AX and cellulose (blue) in cell walls. Low substituted lsAX (red) self-aggregates, and binds more to cellulose compared to high substituted hsAX (green).

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Scientific Achievement

A molecular-level description of how arabinose side-chains affect xylan properties was obtained. Small-angle neutron scattering (SANS) and high performance molecular dynamic simulations (HPC-MD) were combined synergistically for this study. SANS revealed that increasing arabinose substitution reduces xylan self-aggregation. Simulations explain the SANS result by a decrease in xylan flexibility with arabinose substitution providing new insights into this polymer's function in plant cell walls.

Significance and Impact

Arabinose (Ara) substituted xylans play an important role in the structure and mechanics of plant primary cell walls. Xylan function was studied to determine how chemical composition, specifically the degree of Ara substitution, affect their structural properties. The results suggest highly substituted xylan acts as a spacer, keeping cellulose microfibrils apart, whereas low substitution xylan is localized in plant cell walls and promotes cellulose bundling.

Research Details

- High (hs) and low (ls) substitution arabinoxylan samples were studied using SANS.
- Hamiltonian replica exchange were utilized for HPC-MD

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