Integration of Powder Diffraction and Simulation Required for Accurate Determination of Cellulose Crystallinity

Objective:
• Assess how reliable is the determination of cellulose crystallinity when employing commonly-used powder diffraction methods.

Approach:
• Generate models of cellulose fibrils with varying combinations of crystalline and noncrystalline regions and calculate the corresponding powder diffraction diagrams.

Results:
• Crystalline samples conventionally lead to distinguishable Bragg peaks in the X-ray powder diffraction pattern. However, disorder in cellulose fibrils leads to considerable uncertainty in conclusions drawn concerning crystallinity based on powder diffraction data alone.

• For example, while microfibrils without any crystalline segments can lead to few indentifiable peaks (see p-0 in figures) in powder diffraction diagrams; cellulose microfibrils with both crystalline and non-crystalline segments can lead to data with less identifiable peaks (see p-20). Thus, while powder diffraction is frequently employed to characterize cellulose crystallinity, its interpretation is not straightforward.

Significance:
• Cellulose crystallinity is an important feature affecting enzymatic saccharification of cellulose. A reliable approach for its determination can be based on the combination of powder diffraction and computational methods via calculation of diffraction patterns.

Part of the BER Biofuels SFA at ORNL

Lindner, B.; Petridis, L.; Langan, P.; Smith, J. C., "Determination of cellulose crystallinity from powder diffraction diagrams." Biopolymers 2015, 103(2): 67-73. Contact: smithjc@ornl.gov