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:

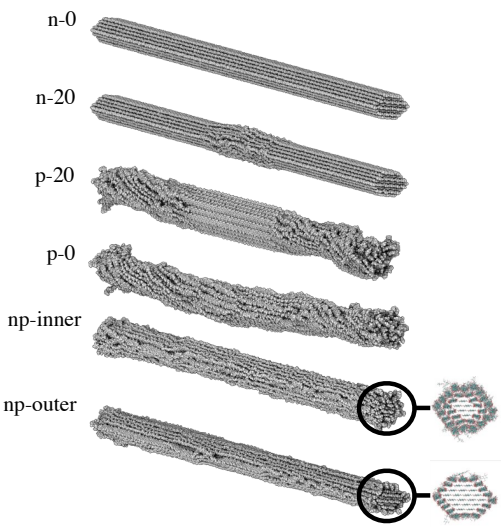
- Generate models of cellulose fibrils with varying combinations of crystalline and noncrystalline regions and calculate the corresponding powder diffraction diagrams.

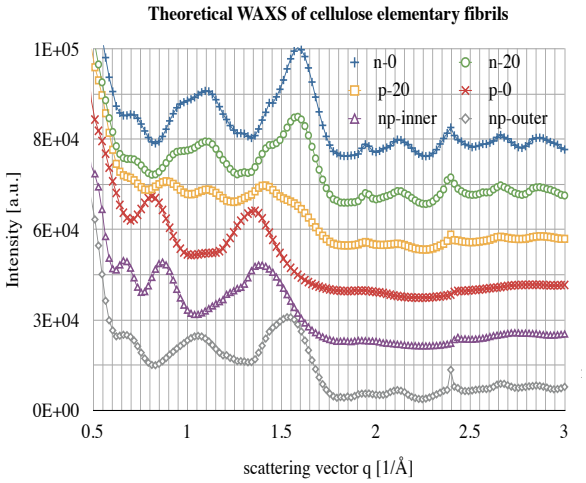
Results:

- 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.





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