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Crystallinity fitting using cellulose crystallite models

P. Ahvenainen[1], R. Serimaa[1]
[1]*University of Helsinki, Department of Physics, Helsinki, Finland*

Cellulose is the most abundant biopolymer on Earth and hence it has enormous potential as a source of renewable energy. The nanoscale properties of cellulose are also import for the wood and papermaking industries. The atomic level structure of naturally occurring cellulose Iβ allomorph is well known [1] and this atomistic model is employed in this study for the cellulose unit cell structure. The cellulose crystallinity cannot be measured directly with scattering methods, but the crystallinity of the sample can be estimated by fitting models of crystalline and amorphous contributions to the sample intensity profile. The crystallinity fitting can be enhanced by improving the cellulose fitting model or the amorphous model. We focus on the cellulose crystallite model. The nanoscale level organization of crystalline cellulose in different plant materials is less well established that the unit cell structure of cellulose Iβ. Information on the texture of the sample is obtained efficiently by measuring the sample with a two-dimensional detector. The two-dimensional diffraction pattern can be used to obtain a wealth of information in one measurement, including the crystallite size, crystallite orientation and the crystallinity of the sample. The small size of cellulose crystallites in the wood cell wall limits the information obtainable from the diffraction pattern as the diffraction peaks widen and overlap. The overlapping of certain diffraction peaks can be studied at least qualitatively by computing the diffraction patterns from crystallite models of varying dimensions. Different models for cellulose crystallite have been suggested in the literature, such as the 36 chain model [2]. We investigate how the crystallinity fitting is influenced by the selected cellulose crystallite model and evaluate the suitability of different models to experimental X-ray scattering data of plant material, wood and highly crystalline cellulose.

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