Supplementary information

Identifying multiple forms of lateral disorder in cellulose fibres

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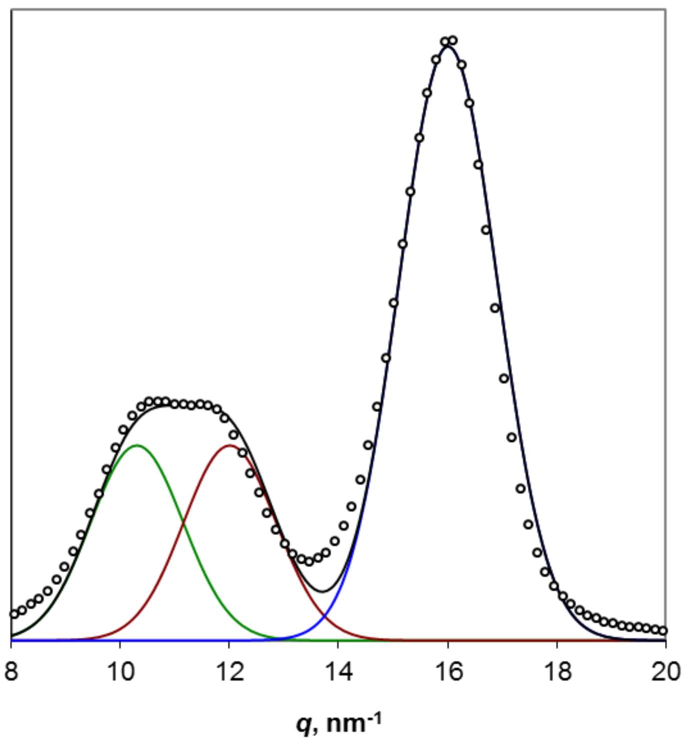
Many strong biological materials exist in the form of fibres that are partially crystalline but contain a substantial proportion of disordered domains, which contribute to the mechanical performance but result in broadening of the reflections in the diffraction patterns of such materials and make structure determination difficult. Where multiple forms of disorder are simultaneously present, many of the accepted ways of modelling the influence of disorder on a fibre diffraction pattern are inapplicable. Lateral disorder in cellulose fibrils of flax fibres was characterized by a multi-step approach. First, a scattering component derived from domains less uniformly oriented than the rest was isolated. A second scattering component giving rise to asymmetry in the radial profiles of the equatorial reflections was then quantified and subtracted. This component was associated with domains that could be related to the crystalline cellulose lattice, but with more variable and, on average, wider equatorial d spacings. A further partially oriented component with highly disordered lateral d spacings unrelated to any of the cellulose lattice dimensions was identified. This component may be derived from non-cellulosic polysaccharides. The remaining broadening was then separated into a contribution from disorder within the crystalline lattice, including known disorder in hydrogen bonding, and a Scherrer contribution from the microfibril diameter. The methods described are likely to find applications in the study of both natural and synthetic polymer fibres in which mechanical properties are influenced by disorder.



Supplementary Figure 1. Fitting of symmetrical (Gaussian) functions to the radial profiles of the 1-10 (green), 110 (red) and 200 (blue) reflections.