MS87.O02

Unravelling the nanostructure of cellulose microfibrils

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Cellulose is the most abundant naturally occurring polymer and has diverse applications in biology, energy and engineering. The cellulose nanostructure has implications on the mechanical strength of natural materials such as wood and nanocelluloses are also being used to create high-performance composite materials with properties comparable to aramid fibres and carbon nanotubes. The efficiency of breakdown of cellulose into ethanoic alcohols for biofuels is also strongly linked to the aggregation of cellulose fibres into microfibrils. Despite this, the nanostructure of cellulose microfibrils is not well understood. Neutron scattering is a powerful way to distinguish order and disorder in biological fibres, wherever the disordered regions are accessible to deuterium exchange. The aggregation of microfibrils in plant cell walls, coupled to the benefits of deuterium exchange and increased scattering contrast using neutrons gives rise to a small-angle Bragg reflection allowing the size of microfibrils to be deduced. Applying these measurements with a range of spectroscopic techniques and wide-angle X-ray and neutron scattering (WAXS, WANS) has enabled us to develop a model for the structure for the microfibrils of cellulose microfibrils in a range of plant species. The scattering data were consistent with 3nm fibrils with both hydrophobic and hydrophilic surfaces exposed. Disorder in chain packing and hydrogen bonding were shown to increase outwards from the microfibril centre. Axial disorder could be explained in terms of twisting of the microfibrils, with implications for their biosynthesis. The disorder aspects of these microfibrils are directly related to the mechanical strength of wood and the natural variation in microfibril angle reflects this. We will present the outcome of in-situ stretching measurements of cellulose microfibrils with insights into the mechanism of the absorption of strain to further probe this mechanical strength.

Keywords: cellulose, fibre diffraction