X-ray diffraction as a tool to study the arrangement of cellulose molecules in plant cell walls

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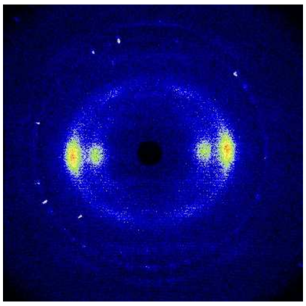
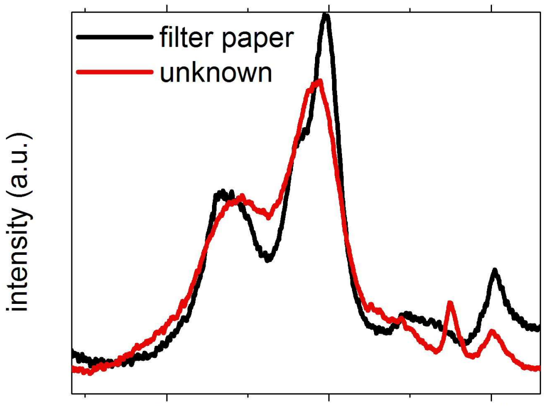
Cellulose, the primary structural polymer in plant cell walls, is unique among polymers utilised by man in its simultaneous synthesis of the polymer and primary unit of nanoscale arrangement, the microfibril. In contrast with the technological world, the plant kingdom achieves diverse mechanical functionality simply by modulating the nanoscale arrangement of cell wall polymers, by the arrangement of cellulose microfibrils. Because of its suitability for spatially localised *in situ* measurements, we have used wide angle x-ray diffraction (WAXD) patterns to investigate the nanoscale arrange of cellulose in microfibrils (Garvey *et al.*, 2005; Garvey *et al.*, 2006) and in oriented samples with respect to applied forces (Martinschitz *et al.*, 2006). Microfibrils are composed of an integral number of cellulose chains, and the number and thus the size of the microfibril are characteristic of the botanical origin of the cellulose. These studies apply a pure size broadening approach to the interpretation of cellulose X-ray diffraction peaks (Garvey *et al.*, 2005). Here we report WAXD area detector data, shown in the image, from plant material presumed to be the gut contents of an extinct giant marsupial, *Diprotodon opatum,* excavated from Lake Callabonna, South Australia (Stirling, 1894).



The two-dimensional anisotropic WAXD data has been radially averaged around the x-ray, centre of the image, to produce a one-dimensional representation, shown in the graph. Using a Voigt function to approximate size broadening of cellulose diffraction peaks we speculate on the putative diet of this animal, based on comparison with size broadening of diffractions peaks of material from modern plants (from the same region), and other sources of cellulose. While these observations give clues to the diet of this giant extinct marsupial, they also give interesting insights into the interpretation of WAXD from cellulose, and ultimately will help us exploit this renewable and versatile material, cellulose.



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Martinschitz KJ, Boesecke P, Garvey CJ, Gindl W & Keckes J. (2006) *Journal of Material Science*, DOI: 10.1007/s10853-006-1237-7.
Stirling EC. (1894) *Nature*, **50:** 184-188.