

## NEUTRON AND SYNCHROTRON X-RAY FIBER DIFFRACTION STUDIES OF CELLULOSE POLYMORPHS

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We are determining the precise crystal structures and H-bonding systems of naturally occurring and processed cellulose polymorphs. Methods have been developed for obtaining oriented polycrystalline fibers that diffract X-rays and neutrons to atomic resolution. <sup>1</sup> For the first time, data have been collected from naturally occurring pure cellulose I $\beta$  isolated from *Glaucozystis* (a microalgae) and from pure cellulose I $\alpha$ , isolated from *Tunicate* (a small sea creature). We have also collected data from the polymorphs resulting from cellulose processing; II (both mercerized and regenerated), III(I) and III(II). <sup>2,3</sup>

Synchrotron X-rays are providing accurate crystallographic parameters for C and O atoms. <sup>4</sup> However, because of the relatively weak scattering power of H atoms for X-rays, neutrons are used to determine their parameters. We have developed methods for replacing labile H atoms with D, without any loss in crystalline perfection. <sup>5</sup> Deuterated fibers can diffract neutrons with intensities that are substantially different from the intensities collected from hydrogenated fibers. Measured intensities <sup>6</sup> are used to compute Fourier difference maps leading to a full description of the H-bonding systems. <sup>7</sup>

These studies are carried out at the European Synchrotron Radiation Facility and the high flux reactor run by the Institut Laue Langevin in Europe. However, a neutron diffraction station has just been built at LANSCE, Los Alamos National Laboratory, which will allow, for the first time, similar studies of polymers to be carried out in the USA. <sup>8</sup>

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