



SIMPOSIO INTERNACIONAL SOBRE MATERIALES LIGNOCELULOSICOS

A SIMPLIFIED UNDERSTANDING OF CELULOSE X-RAY CRYSTALLINITY

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ABSTRACT

X-Ray diffraction is often used to study cellulosic materials, which are often composed of small crystals whose structures depend on the history of the sample. Many properties of cellulose are related to the particular crystalline form and to the degree of perfection of the crystals. However, there is substantial confusion. Several conventions have been used to describe the unit cell and Miller indices for the different peaks. Therefore, adoption of a single convention is urged, one that is also used in the determinations of atomic coordinates of cellulose structures. In turn, the coordinates can be used to calculate diffraction patterns using free software. Models can be either based on a unit cell and infinite but of varied size, or they can explicitly include all the atoms in a model that is, for example, twisted. Much of the intensity that is often attributed to “amorphous” material is simply overlap of broad peaks simulated from small model crystals.