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Possibilities of proton magnetic resonance in determination the cellulose crystallinity

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Abstract

A layered model of the structural organization of macrofibrils of native cellulose, consisting of microfibrils, which include elementary fibrils, has been developed. A feature of the proposed model is the presence of slit-like pores between the crystalline elements of cellulose. It was found that, on average, each water molecule interacts with one glucose residue of the surface chains of cellulose with the formation of hydrogen bonds in the framework of monolayer adsorption. This allows to establish a correlation between the cellulose crystallinity and the capacity of the adsorption water monolayer on its active surface. Based on the condition of rapid molecular exchange between the adsorption water layers in the framework of the Bloembergen-Purcell-Pound theory, an approach is proposed for determination the capacity of water monolayer. The obtained values are consistent with the results of solving the Brunauer-Emmett-Teller equation for the adsorption isotherm of water on the active surface of cellulose. The Fourier transform of the free induction decay signal of cellulose allows to estimate its crystallinity at various moisture contents. Methods have been developed for assessing the crystallinity of different types of dry cellulose based on NMR relaxation parameters — spin-lattice relaxation time and spin-spin relaxation time. Using the method of deuteration of cellulose, the relaxation times of its crystalline regions were determined. The results of preliminary studies showed that the crystallinity of cotton cellulose is higher in comparison with the same parameter of woody types of cellulose. A comparison of the literature and the data we obtained using ^{1}H-NMR relaxation confirmed the possibility of utilizing the developed methods to solve the tasks of scientific research and conducting quality control of cellulosic materials at specialized enterprises.

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