

## The nature of the supramolecular rearrangements of native cellulose in the process of enzymatic hydrolysis

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### Abstract

Based on the theories of NMR relaxation in multiphase systems and adsorption phenomena, methods is developed for determining the degree of crystallinity, specific surface area, and the average transverse size of native cellulose crystallites. In particular, using the Bloembergen-Purcell-Pound theory and the condition of fast exchange, a relation is obtained for determining the monomolecular adsorbed layer. A correlation is established between the capacity of the monolayer and the degree of crystallinity of the sample under study. This took into account the fact that the content of water molecules in the monolayer is equivalent to the number of glucopyranose rings in the surface chains of the cellulose, which made it possible to associate the capacity of the monolayer with the degree of crystallinity of the sample. Within the framework of modern ideas about the layered organization of elementary cellulose fibrils and about their entry into the structure of microfibrils, a technique is developed for estimating the average transverse dimensions of cellulose crystallites using an experimentally determined degree of crystallinity. It is established that sequential chemical treatment of the native starting cellulose with alcohol, ether and alcohol, ether and urea leads to a significant decrease in the degree of crystallinity, an increase in the specific surface. It is assumed that this effect should be associated with the weakening of intra-, intermolecular hydrogen bonds of cellulose under the action of these reagents. It is shown that preliminary chemical treatment of cellulose samples significantly affects the efficiency of its enzymatic degradation. Obviously, during the interaction with cellulose, the enzymatic complex switches its intra- and intermolecular hydrogen bonds of the -O-H..O type and neutralizes the interlayer hydrogen bonds of the -C-H..O type. It is confirmed that the main component of the cellulase complex, *endo*-1,4- $\beta$ -glucanase, produces the greatest changes in the structure of cellulose.

### References

- [1] Y.B. Grunin [et al.] Features of the sorption of water vapor and nitrogen on cellulose. *Russian Journal of Physical Chemistry A*. **2013**. Vol.87. No.1. P.100-103.
- [2] NMR analyzer «Spin Track». URL: <http://www.nmr-design.com>.
- [3] V.I. Chizhik. Nuclear magnetic relaxation. *St. Petersburg: SPbSU*. **2004**. 385p. (russian)
- [4] Y.B. Grunin. Analysis of the cellulose-water system by modified methods of proton magnetic resonance: Doctor's thesis. *Riga*. **1989**. 452p.
- [5] Y.B. Grunin [et al.] Features of the structural organization and sorption properties of cellulose. *Polymer Science Series A*. **2015**. Vol.57. Iss.1. P.43-51.
- [6] Y.B. Grunin [et al.] Features of Dispersing of Crystalline Cellulose at Its Moistening. *Chemical fibers*. **2017**. No.5. P.31-36. (russian)
- [7] A.A. Klesov, S.Yu. Grigorash Enzymatic hydrolysis of cellulose. *Bioorganic Chemistry*. **1981**. Vol.7. No.10. P.1538-1552.
- [8] M.M. Dubinin New in the Field of Adsorption of Vapors by Microporous Adsorbents. *Journal of Physical Chemistry*. **1987**. No.5. P.1301-1305. (russian)
- [9] Y.B. Grunin [et al.] Supramolecular reorganizations in cellulose during hydration. *Biophysics*. **2015**. Vol.60. No.1. P.43-52.