Abstract (English)

The plant cell wall is a highly ordered and specialized network, formed mainly of polysaccharides, glycoproteins, phenolic compounds, minerals and enzymes. Being the most widespread and probably the most complex structural network in Nature, the main functions of plant cell wall are relatively clear - determination of plant morphogenesis, architecture, management of mechanical responses, strength, flexibility, growth management, defense responses, intercellular communication etc. Despite the inconsistency of the relationships between structure and properties of plant cell wall, which has been debated since the late 1960s, the role of cellulose-hemicellulose interactions with respect to mechanobiology of plant cell wall is undisputed. Modern theory supports the notion that cellulose is the main load-bearing component of plant cell wall, while the key component of plant cell wall mechanical properties - interfiber adhesion - is determined by the hemicellulose-mediated interactions.

Despite recent progresses, there is still much to consider on physicochemical properties of plant cell wall polysaccharides and the mechanical properties of plant cell wall. But how can the respected results be achieved? Plant cell wall may be studied directly by either decomposition of its constituents in plant cell wall (in muro), inhibition of biosynthesis, in vitro solubilization or chemical modification. However, evaluation of the mechanical properties of plant cell wall is severely limited by the experimental techniques used, making the results variable and context-dependent. Sample processing is also challenging in single-cell studies, and even when processed, results are mainly site-dependent. The development of plant cell wall analogues of interconnected bacterial cellulose and plant cel wall hemicelluloses can serve as a tool to achieve a simplified macroscale representations of plant cell wall that have a homogeneous structure and are repeatable. Such an approach has already made possible to catalogue the effects of the main plant cell wall polysaccharides on the structure and mechanical properties of the plant cell wall analogues and to define the mechanisms of polysaccharide interaction with cellulose. However, conventional laboratory techniques are struggling to allow the determination of the interfiber adhesive forces, which is undisputedly crucial for the mechanobiology of plant cell wall. In silico numerical modeling allows to approximate the structure and mechanical properties of plant cell wall with respect to introduced composition, spatio-temporal parameters, and physicochemical properties of plant cell wall polysaccharides introduced. It also allows to reach promising insights on network structure and mechanics with regard to its formation, density, location and strength of cellulose-hemicellulose junctions as well as the nature of the role of other plant cell wall polysaccharides.

In current Ph.D. Thesis, all the crucial theoretical background regarding mechanical properties of bacterial cellulose, hemicelluloses (xylan, arabinoxylan, xyloglucan, and glucomannan), their binary (bacterial cellulose-hemicellulose) and ternary (bacterial cellulose-hemicellulose-pectin) composites has been gathered, and discussed with respect to the type of specific polysaccharides, their origin, production methods, applied treatment, as well as various methodological approaches to the biosynthesis of bacterial cellulose.

In the following part of current Ph.D. Thesis, theoretical explorations have been focused on the exploration of an existing numerical models of plant cell wall regarding the network fine structures, its supramolecular properties and polysaccharide binding affinities. For this purpose, extensive revision of an existing concepts of plant cell wall structure has been also conducted, allowing to incorporate certain physical and biomechanical aspects of cell wall architecture to the understanding of the mechanisms, which allow to control cell wall mechanical responses.

In the next stage of the following research, mechanical and molecular properties of bacterial cellulose-hemicellulose plant cell wall analogues were investigated to determine the effect of physicochemical properties of various hemicellulose polysaccharides (xylan, arabinoxylan, xyloglucan and glucomannan) on overall performance of bacterial cellulose-hemicellulose plant cell wall analogues in terms of elastic and plastic responses. Current research supported an idea that mechanical properties of bacterial cellulose-hemicellulose plant cell wall analogues are determined predominantly by the deformation of cellulose fibers, mediated by hemicelluloses. While elastic deformation of bacterial cellulose-hemicellulose plant cell wall analogues is determined by stretching vibrations of the structural bonds of cellulose and hemicelluloses, plastic deformation is defined by the supramolecular changes occurring within the structure of bacterial cellulose-hemicellulose plant cell wall analogues.

The following part of current Ph.D. Thesis was focused on establishing of the numerical model of bacterial cellulose-hemicellulose plant cell wall analogues following the principles of coarse-grained molecular dynamics, with fibers modelled using the bead-spring approach. To validate the model and explain the structural and mechanical role of hemicelluloses, bacterial cellulose was synthesized in the presence of different concentrations of xylan, arabinoxylan, xyloglucan, or glucomannan and subjected to nano- and macroscale structural and mechanical characterization. The data obtained were used to interpret the effects of each hemicellulose on the mechanical properties of bacterial cellulose-hemicellulose plant cell wall analogues based on the sensitivity of the model. Current part of the work showed an agreement between simulated networks and synthesized plant cell wall analogues. It was observed that mechanical properties of bacterial cellulose–hemicellulose plant cell wall analogues are not determined by the deformation of hemicelluloses itself, but mainly by the deformation of cellulose fibers, mediated by hemicelluloses. Such a mediates, conceptually similar to biomechanical hotspots occurring in muro, change the force of interfiber interaction, being the main factor affecting the mechanical properties of bacterial cellulose– hemicellulose plant cell wall analogues. In addition, force of interfiber interaction is also defined by the morphological features of bacterial cellulose–hemicellulose plant cell wall analogues, such as fiber width/length/modulus. It was also shown that mechanical properties of bacterial cellulose–hemicellulose plant cell wall analogues correspond to those of simulated networks, confirming applicability of the latter for the exploration of the mechanobiology of cellulose–based fiber networks.

As a supplementary research, exploration of the effect of hemicellulose–specific enzymes on the structure and mechanical performance of bacterial cellulose–hemicellulose plant cel wall analogues was conducted. Current research supported showed that hemicelluloses, incorporated in bacterial cellulose fiber network exist as both enzyme–accessible and enzyme–inaccessible. It results in enzyme–inaccessible hemicelluloses are defining trends on data change of the mechanical properties of the respected plant cell wall analogues, while enzyme–accessible hemicelluloses are defining data fluctuation.

Keywords: bacterial cellulose, hemicellulose, plant cell wall analogues, mechanical properties, molecular dynamics simulation.