Pectin is the most structurally complex family of polysaccharides in nature. Among popular fruits, pears, apples as well as citrus fruits contain large amounts of pectin, while soft fruits like cherries, grapes, and strawberries contain small amounts of pectin. Pectin is abundant in walls that surround growing and dividing cells, walls of cells in the soft parts of the plant and in the middle lamella. Due to numerous interesting properties arising from complex nanostructure and their potential applications in pharmaceutical, food and material industry, pectins have been a subject of many bio-molecular studies.

Recently, in the Department of Microstructure and Mechanics of Biomaterials in the Institute of Agrophysics PAS, it was discovered that in fresh fruits and vegetables such as carrot, apples or pears, diluted alkali soluble fraction of pectin (DASP) form regular interlinked network on mica. This regular structure would have a great importance for cell wall integrity and therefore texture and firmness of the whole fruits and vegetables. This hypothesis was supported by visible degradation of the network for pectins extracted after storage. However, at present neither the mechanism of networking nor molecular structure of this pectin fraction is not known yet.

The goal of this research is to identify the underlying structural composition and mechanism responsible for self-assembly phenomenon of diluted alkali soluble fraction extracted from plant cell wall pectins. The considerable progress in understanding the above described mechanisms and outgoing properties of the diluted alkali soluble pectins (DASP) might be achieved by means of the modern experimental and theoretical methods, such as atomic force microscopy (AFM) and computational chemistry. The research scope of this proposal has an original character and combines both, experimental and theoretical work (namely numerical modelling) to identify the underlying structural composition and mechanism responsible for self-assembly phenomenon of diluted alkali (sodium carbonate) soluble fraction of pectins. The initial phase of this study is focused on experimental examination of DASP fraction. This task will involve enzymatic modification of pectins and observation of the results of chemical modification using the atomic force microscopy. The theoretical basis of the observed phenomena will be carried out on the basis of numerical modeling techniques (density functional theory - DFT and molecular dynamics - MD). First tasks of numerical study will be focused on proper definition of pectin “building blocks” – oligomers of individual carbohydrates. Then we will proceed to study the interactions between biopolymers, exploration of possible configurations and their stability. Further studies of the structural composition of DASP will be extended to include behavior of the DASP fraction in water solutions and interactions with other DASP molecules in large scale assemblies.

The proposed research project based on AFM imaging of polysaccharides molecules combined with computational chemistry provide new approach to studying localized pectin structure that may increase our knowledge of the biological functions and functional properties of pectin. Plant pectin is considered to be one of the major contributors for maintaining the texture of fruits and vegetables. Other known functions of pectin in plant include growth, morphology, development , and plant defense. In food industry pectin in known as a dietary fiber, which is helpful in maintaining good digestive health. The ability of pectin to form gels in water solutions makes it an important food component for gastronomy and food industry. The impact of the project results on food design will be achieved by understanding the fundamentals of specific pectins gelation rate and gelling properties which arise from their molecular sturcture. We believe that this research will also significantly contribute to the state of the art in the mathematical modelling of hierarchically structured biological materials such as plant cell walls and tissues.