The objective of antifreeze proteins (AFPs) is to protect fluids contained in a bodies of living organisms from the freezing, when the ambient temperature falls below zero degrees Celsius. Crystals of ice which form during freezing, as well as increasing volume of water, rupture the cells membranes and (by destroying their structure) cause death of cells. Antifreeze protection is based on the keeping of body fluids in the supercooled state. Widely accepted mechanism of action of AFPs assumes that molecules of protein are able to adsorb on the surface of ice crystals, that are formed inside the organism, which prevents them from growing.

Despite the effort of researchers, the manner in which antifreeze proteins are able to recognize crystals of ice when they are surrounded by large excess of supercooled, but still liquid, water is still not fully understood. It appears that solvation water of AFPs may play a significant role in this process. The structure of solvation water of the active region of antifreeze proteins is noticeable different from the structure of water located in the vicinity of a remaining regions of the protein surface and shows similarities to the structure of ice. This effect can - on the one hand - facilitate the freezing of water located between the protein and ice, leading to irreversible binding, and on the other enable the differentiation between water in the solid and liquid state, which is necessary for the protein to perform its function.

The aim of the proposed research is to investigate the structure and the role of solvation water of antifreeze proteins in the process of the binding of those proteins with the surface of ice. In order to do that, computer simulations of systems consist of the crystal of ice and a selected AFP, separated by the layer of a liquid water, will be conducted. Research will be performed for several temperatures within the range of 250 – 270 K and for several distances between the molecule of protein and ice. The analysis of the obtained results will include the structural properties of the solvation water of the active site of AFP and of water located in the immediate vicinity of the crystal of ice.

Obtained results will allow for a better understanding of the details concerning the process of the freezing of water located in the region between AFP and the crystal of ice. It will be the next step in the way of knowing the role of the solvation water in the process of the binding of antifreeze proteins with ice and of understanding the mechanism of action of these proteins.