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Molecular dynamic simulation on the interaction between ‘antifreeze’ polypeptide, water and an ice

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The inhibition of ice growth is an important issue in various fields, such as the maintenance of the quality of food texture in food preservation, and cryosurgery. Antifreeze protein (AFP) and antifreeze glycoprotein (AFGP) have been investigated in relation to the inhibition of ice growth. This is because the AF(G)P solutions have the following properties: (a) the freezing point drops noticeably, (b) the melting point is retained, (c) the osmotic pressure does not significantly increase, and (d) specific facets are observed on the surfaces of ice crystals. Therefore, AFP and AFGP are promising additives for the applications. On the other hand, the denaturation of these proteins occurs inevitably. Also, these proteins are expensive regardless of synthetic one or natural one. Kun and Mastai (Peptide Science, vol. 88, 2007, pp. 807-814) synthesized a twelve-residue polypeptide based on a part of winter flounder AFP. They showed that this polypeptide has the aforementioned two properties; (a) and (b). Our research group expects that denaturation of the polypeptide does not occur in this case because the short helical structure of the polypeptide, which includes many hydrophobic residues, is maintained with strong hydrophobic interaction and the hydrogen bonds. However, as far as the present authors know, no report has been published concerning the mechanism of ice-growth inhibition for the polypeptide.

Thus, we have carried out molecular dynamics simulation for the mixture of the polypeptide, water and an ice layer in the present study. We adopted the Canonical ensemble. The Newton-Euler equations for the translational and rotational motions of the molecules were solved at each time step, and were integrated with respect to time by using the Gear algorithm. The TIP4P/Ice potential function was used for the interaction between two water molecules. The Ewald method was used for the Coulomb potential in order to reduce the electrical force of distant molecules. The OPLS parameters were adopted as the potential parameters of each site of the peptide. The results of the simulations showed that the presence of the polypeptide inhibits the hydrogen bonding among water molecules and shortens the period of the hydrogen bonding. Consequently, the presence of the polypeptide attenuated the formation of tetrahedral networks of water molecules near the ice surface. This is a reason for the ice growth inhibition by the polypeptide. When the polypeptide was adsorbed on the ice surface, the motion of the peptide is more noticeable compared with that of the winter flounder antifreeze protein. This is the reason for the necessity of higher concentration of the polypeptide than the winter flounder antifreeze protein for the inhibition of ice growth. All these results are consistent with the experimental results. In addition, we examined the polypeptide bound with hydrophobic glutaraldehyde, which can be a linker of the polypeptide to cooling surfaces. The results showed that the ice growth was further inhibited. It can be concluded that the coating of glutaraldehyde-linked polypeptide might be effective for producing ice-phobic surfaces.

Significance statement

We have carried out molecular dynamics simulation for the mixture of the polypeptide, water and an ice layer in the present study. All the results are consistent with the experimental results. We also examined the polypeptide bound with hydrophobic glutaraldehyde.

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