

Abstract Submitted
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Retardation of ice crystallization by short peptides¹ JUN SOO KIM, ARUN YETHIRAJ, Theoretical Chemistry Institute and Department of Chemistry, University of Wisconsin-Madison — The effect of short peptides on the growth of ice crystals is studied using molecular dynamics simulations. The simulations focus on two sequences (Gly-Pro-Ala-Gly and Gly-Gly-Ala-Gly) that are found in collagen hydrolysate, a substance that is known to retard crystal growth. In the absence of peptides, the growth of ice crystal in the solution with the ice/water interface is observed in at a rate comparable to the experimental data. When peptides are present in the liquid phase, the crystal growth is retarded to a significant extent compared to the pure water. It is found that Gly-Pro-Ala-Gly is more effective (crystallization is up to 5 times slower than in its absence) than Gly-Gly-Ala-Gly (up to 3 times slower) implying that the role of the proline residue is important. The mechanism can be understood in the nature of binding of the peptides to the growing crystal.

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