Correlation between the ice surface structure and the Gibbs-Thomson equation in Molecular Dynamics Simulations

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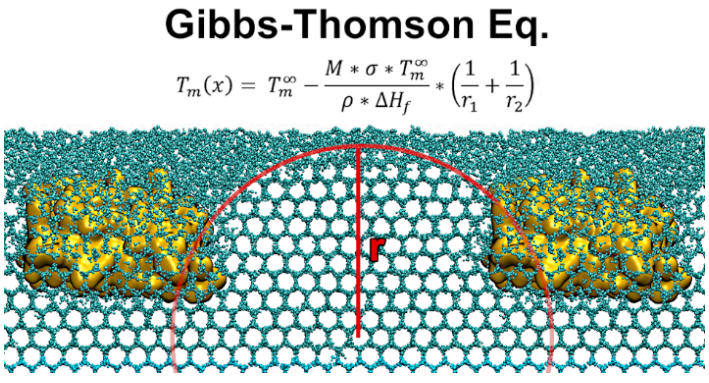
Antifreeze proteins (AFP) are able to influence ice crystal growth and the recrystallization process due to their interaction with the ice crystal. The binding of AFP leads to the formation of a curved ice crystal surface resulting in a melting point depression at this curvature. This is called Gibbs-Thomson effect. It is generally believed that there is a critical radius between the proteins on the ice surface that determines the maximum thermal hysteresis. In this work, molecular dynamics simulations were used to analyze the resulting structure of the ice crystal surface after adsorption of an AFP. Contrary to assumption in literature, it could be shown that the critical radius is not directly between the adsorbed proteins. Furthermore, we have shown that the minimum temperature at which the system does not freeze is in very good agreement with the value calculated with the Gibbs-Thomson equation at the critical radius, provided that dynamic system conditions are taken into account. This proves that the Gibbs-Thomson effect is the basis of ice crystal growth inhibition and that molecular dynamics simulations are useful for predicting melting point depression by AFP.



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