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Effect of latent heat of crystallization on morphology of ice crystal grown from undercooled water

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It has been known that the ice crystal growth from undercooled water is affected in the presence of biological proteins. Typical examples of the biological proteins are antifreeze proteins (AFPs) and ice-nucleating proteins (INPs). The mechanisms how these proteins modify the growth processes of ice crystals have been unknown. Recently, in-situ observation of an ice crystal grown from undercooled liquid water mixed with INPs (Xanthomonas Campestris [1]) was carried out [2]. The results showed that the existence of the INPs decelerated growth in the c-axis direction, whereas accelerated growth in the a-axis direction. This means that the morphology of ice crystal is modified in the presence of the INPs. However, the reason why the INPs affect the growth of ice crystals still remains unclear.
The purpose of this study is to evaluate the effect of the local temperature increase by release of latent heat of crystallization on the morphological change of ice crystal. When the INPs inhibit the growth in a certain direction, the release of latent heat will decrease in total. As a result, it is expected that the growth in the different directions can be promoted.
We carried out the numerical simulations of ice crystal grown from undercooled water in the presence of the INPs. We consider the growth in the a- and c-axes directions (two-dimension). We adopt the phase-field model [3], which takes into account the following physical processes; local temperature increase associated with crystallization, unsteady thermal diffusion, and crystal growth speed depending on undercooling at crystal-melt interface. We assumed that the INPs inhibit the growth in the c-axis direction because of the binding of INPs to a basal plane of ice crystal. The effect of growth inhibition is taken into account in our numerical model by reducing the kinetic coefficient in this direction artificially. Our numerical simulations showed that the growth in the a-axis direction could be promoted by the growth inhibition in the c-axis direction. We also investigated the dependence on undercooling of water. It was found that the growth promotion in the a-axis direction is remarkable at larger undercoolings than at lower ones. From these numerical simulations, it was suggested that the crystal growth in a certain direction can be promoted in the presence of the INPs, which inhibit the growth on the specific crystallographic plane. This might be an important effect for determining the morphology of ice crystal grown from undercooled water.

References:
[1] Wilson et al., Env.Microbiol. 8, 1816 (2006). [2] Nada et al., in prep. [3] Wang et al., Physica D 69, 189-200 (1993).

Keywords: ice crystal, morphology, protein molecules, recalescence, numerical simulation