Free Energy Barriers for Anti-Freeze Protein Engulfment: A Model for the Effects of Supercooling, Footprint Size, and Spatial Separation

Hossam Farag[§], Baron Peters[||,†,*]

[§] Nuclear, Plasma, and Radiological Engineering, University of Illinois at Urbana–Champaign, Urbana, IL 61801
[||] Chemical and Biomolecular Engineering, University of Illinois at Urbana–Champaign, Urbana, IL 61801[†] Department of Chemistry, University of Illinois at Urbana–Champaign, Urbana, IL 61801
*Corresponding author: baronp@illinois.edu

ABSTRACT: Biological anti-freeze proteins (AFPs) protect organisms at freezing conditions by attaching to the ice surface and arresting its growth. In the theory of DeVries et al., each adsorbed AFP locally pins the ice surface, resulting in a metastable dimple for which the interfacial forces counteract the driving force for growth. As supercooling increases, these metastable dimples become deeper until metastability is lost in an "engulfment" event where the ice irreversibly swallows the AFP. Engulfment resembles nucleation in some respects, and this paper develops a model for the "critical profile" and free energy barrier for the engulfment process. Specifically, we develop a variational model for the ice-water interface and obtain estimates of the free energy barrier as a function of the supercooling, the AFP footprint size, and the distance to neighboring AFPs on the ice surface. We discuss how this information might be used to predict thermal hysteresis properties as a function of AFP properties and AFP coverage.