Microscopic ordering of supercooled water on the ice basal face

Growth of ice crystals is ubiquitous around us, but we still do not know what is occurring at the forefront of crystallization. In general, the interfacial structure is inseparably involved in the microscopic ordering during crystal growth. However, despite its importance in nature and technology, the intrinsic role of the interfacial structure in the melt growth of ice remains to be elucidated. Here, using extensive molecular dynamics simulations, we comprehensively explore how supercooled water molecules are incorporated into the ice basal face. Structural and dynamic characterizations of the ice-water interface demonstrate that the ice basal face is sharp at the molecular level and its growth proceeds layer-by-layer through two-dimensional nucleation without any intermediate structures. We further quantify the crossover from layerwise to adhesive growth, called kinetic roughening, with the height difference correlation and the normal growth rate analysis. Moreover, we identify the presence of an ultra-low density water layer in contact with the structural interface, which assists two-dimensional nucleation at a small amount of supercooling without involving any triggers, such as dislocations.[1]

[1] K. Mochizuki*, K. Murata*, and X. Zhang, “Microscopic ordering of supercooled water on the ice basal face”, under review