Towards understanding heterogeneous ice nucleation on realistic silver iodide surfaces from atomistic simulation

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Small particles of silver iodide (AgI) are known to have excellent ice nucleating capabilities and have been used in rain seeding applications. It is widely believed that the silver terminated (0001) surface of β-AgI acts as a template for the basal plane of hexagonal ice. However, the (0001) surface of ionic crystals with the wurtzite structure is polar and will therefore exhibit reconstructions and defects. Here, we use atomistic molecular dynamics simulations to study how the presence of defects on AgI(0001) affects the rates and mechanism of heterogeneous ice nucleation at moderate supercooling at -10 ºC. We first consider AgI(0001) surfaces exhibiting vacancies, step edges, terraces, and pits, and compare them to simulations of the corresponding ideal surface. We find that, while point defects have no significant effect on ice nucleation rates, step edges, terraces, and pits reduce both the nucleation and growth rates by up to an order of magnitude, which can be understood from the atomistic details extracted from the simulations. The reduction of the ice nucleation rate correlates well with the fraction of the surface area around the defects where perturbations of the hydration layer hinder the formation of a critical ice nucleus. Finally, we consider more realistic AgI(0001) surfaces with 5x5 surface reconstructions that cancel the surface dipole, and report on their ice nucleating abilities.