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Effect of defects on heterogeneous ice nucleation at silver iodide surfaces

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Silver iodide (AgI) is an excellent ice-nucleating agent, which is widely used in cloud seeding [1]. The ice-nucleating efficacy of crystals is related to their specific crystallographic features. However, our knowledge of the microscopic mechanisms responsible for the ice-forming properties of different materials is relatively limited. Previous theoretical work has shown that ice nucleation on AgI occurs on time scales accessible to unbiased molecular dynamics simulations [2], unlike in many other systems relevant for heterogeneous ice nucleation in the atmosphere, which makes this material a good benchmark system.

In this study, we investigate the ability of non-ideal AgI surfaces to nucleate and grow ice, using molecular dynamics simulations with the TIP4P/ice model of water [3] and AgI/water interactions proposed by Hale and Kiefer [4]. We present simulations on AgI surfaces exhibiting point defects, step edges, pits, and terraces, and compare them to simulations of the ideal, flat β-AgI (001) surface. None of the defects considered were found to further promote the growth of ice on AgI, and ice nucleation was always observed to originate in the ideal region of the surface. We present and discuss the different ice nucleation and growth rates, as well as the atomistic details of the nucleation and growth mechanism, for the AgI surfaces considered in this work.

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