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Effect of surface geometry on heterogeneous ice nucleation

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Understanding the way in which ice forms is of great importance to many fields of science.
Pure water droplets in the atmosphere can remain in the liquid phase to nearly -40º C. Crystallization of ice in the atmosphere therefore typically occurs in the presence of aerosol particles, such as mineral dust, soot or organic particles. These ice nucleating particles (INPs) trigger heterogeneous ice nucleation at clearly higher temperatures. Therefore, a better understanding of how the various types of aerosol particles present in the atmosphere affect ice nucleation (IN) in clouds would be an important advance in the field of atmospheric science.

Experiments have shown in great detail what is the IN activity of different types of compounds, and recently also clarified the importance of small surface features such as surface defects. The molecular-scale processes responsible for ice nucleation are still not well known, however, and difficulties in atomic-scale characterization of complex and imperfect surfaces means that a full understanding of these processes from solely experimental evidence is still a distant goal. In recent years, several computational studies have been published on heterogeneous ice nucleation, advancing our understanding of the details of ice nucleation in many materials. The role of defects has been studied less, but recently the importance of feldspar microstructure and different crystallographic faces of feldspar were shown to be responsible for IN activity of feldspars (Kiselev et al., 2017). Simulations also showed enhanced ice nucleation efficiency in confined geometry such as wedges or pits (Bi, Cao and Li, 2017).

We are studying these topics by utilizing the monatomic water model (Molinero and Moore, 2009) for unbiased molecular dynamics (MD) simulations, where a surface including defects, such as pyramidal pits, steps or surface cracks, immersed in water, is cooled continuously below the melting point over tens of nanoseconds of simulation time and crystallization is followed.

Results of simulations on pyramidal pits on Si (100) surfaces, for example, show a clear ($\Delta T > 10$º C) enhancement of ice nucleation compared to flat Si (100) or Si (111) surfaces. Understanding the enhanced activity in such confined geometry may lead to characterization of active sites on some ice nucleating materials, as well as to development of optimal cloud seeding materials.

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