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Ice nucleation in confined geometry and the role of latent heat

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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 -40 ºC. Crystallization of ice in the atmosphere therefore typically occurs in the presence of ice nucleating particles (INPs), such as mineral dust or organic particles, which trigger heterogeneous ice nucleation at clearly higher temperatures. Such active INPs can also be used for rain enhancement.

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. In recent years, several computational studies have advanced our understanding of the details of ice nucleation in many materials, and also the role of defects. Recently simulations 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 system including a defected surface, 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, an experimentally realizable system, show a clear ($\Delta T > 10$ ºC) enhancement of ice nucleation compared to flat Si (100) or Si (111) surfaces, in agreement with initial experimental findings of preference of ice to nucleate at these sites. Understanding the enhanced activity in such confined geometry may lead to characterization of active sites on some ice nucleating materials, or lead to designs of new artificial materials optimized for cloud seeding applications.

With a combination of finite difference calculations and molecular dynamics simulations we also show that the release of latent heat from ice growth has a noticeable effect on both the ice growth rate and the initial structure of the forming ice. However, latent heat is found not to be as critically important in controlling immersion nucleation as it is in vapor-to-liquid nucleation [Tanaka et al. 2017].

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