Contribution ID: **38** Type: **Talk**

Enhanced heterogeneous ice nucleation by special surface geometry

Tuesday 9 January 2018 14:05 (20 minutes)

Surface roughness has been long known to affect nucleation, but its role in ice formation remains controversial and poorly understood. Experiments showed ice nucleation is significantly promoted by surface irregularities on hematite, mica, and potassium-rich feldspar, but is relatively insensitive to the roughness of superhydrophobic surfaces.

By employing large-scale, accelerated molecular simulations, here we show that heterogeneous ice nucleation is strongly affected by surface geometry1. An atomically sharp, concave wedge is found to significantly enhance ice nucleation rate by many orders of magnitude over flat surface. However, in contrast to classical nucleation theory, the enhancement is found to occur only under special surface geometries. These include the 70- and 110-degree wedges that match the two intersecting {111} planes of cubic ice lattice simultaneously, thus significantly enhancing the formation of cubic ice. Remarkably, significant enhancement of ice nucleation also occurs when lattice match does not exist, as in a 45-degree wedge. In this geometry, the 45-degree wedge is found to facilitate the formation of special topological defects of ice that subsequently catalyze the growth of regular ice. Therefore, our study not only highlights the active role of defects in nucleation, but also suggests the traditional concept of lattice match between a nucleation center and crystalline lattice should be extended to include a broader match with metastable, non-crystalline structural motifs.

1. Bi, Y., Cao, B. & Li, T. Enhanced heterogeneous ice nucleation by special surface geometry. Nat Commun 8, 15372 (2017).

Significance statement

Traditional wisdom believes a good ice nucleator must be capable of inducing water ordering coherent to ice lattice. We presented the first computational evidence that challenges this understanding by showing ice nucleation can be equally or even more effectively promoted by special surface geometry through inducing a non-crystalline ordering.

Author: Prof. LI, Tianshu (George Washington University)

Co-authors: Mr CAO, Boxiao (George Washington University); Mr BI, Yuanfei (George Washington University)

Presenter: Prof. LI, Tianshu (George Washington University)

Track Classification: Nucleation