4-1-2019

Water Structure and Its Correlation to Heterogeneous Ice Nucleation

Jiarun Zhou
Clemson University

Brittany Glatz
Clemson University

Nurun N. Lata
Michigan Technical University

Sapna Sarupria
Clemson University

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Recommended Citation
Zhou, Jiarun; Glatz, Brittany; Lata, Nurun N.; and Sarupria, Sapna, "Water Structure and Its Correlation to Heterogeneous Ice Nucleation" (2019). Graduate Research and Discovery Symposium (GRADS). 298.
https://tigerprints.clemson.edu/grads_symposium/298

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Heterogeneous Ice Nucleation

Water cycle

Ice on airplane

What affect heterogeneous nucleation rate?

Mineral dust

Heterogeneous ice nucleation?

Mg

2+

Precipitation - mica

promote

Heterogeneous Ice Nucleation

Hexagonal Ice (Water)

Ice

Mineral water

Isotherms of observing ice nucleation at the metastable liquid state

Hexagonal basal plane seed with a radius of 2 nm on K+-mica (a, b, and c) and Mg2+-mica (d, e, and f) at 235 K. Gray: mica surface, cyan: original seed, blue: cubic ice, red: hexagonal ice, ice blue: liquid water, orange: K, green: Mg.

Panel (a) and (d): seed at the beginning of equilibration: panel (b) and (e): growth of ice around seed at the end of equilibration run; panel (c) and (f): growth of ice around seed at the end of 50 ns production run.

Seeds grow differently on K+-mica and Mg2+-mica.

Tilting has been observed to affect the further growth near the seed.

The ability of ion to localize water molecules influences seed growth.

Conclusions and Future Work

• Ion hydration influences water structure. Mg2+ ions have the strongest ability to restructure water in vicinity.

• Further investigation on mechanism of ice nucleation via seeding and water dynamics, along with freezing experiments on different mica systems helps elucidating the role of surfaces in heterogeneous ice nucleation.

References


3. Jiarun Zhou, Nurun N. Latina, Sapna Sarupria, Will Cantrell, to be submitted

Acknowledgement: Palmetto supercomputing @Clemson, National Science Foundation (NSF) Award numbers: AGS-1549388 and AGS-1549384.

Mica Surface

Freshly cleaved muscovite mica contains K+ ions. Washing mica with corresponding solutions can replace K+ with other ions.


Water Adsorption Isotherms

Adsorption isotherms indicates the surface affinity of water. Each data point is composed of eight isotherms at different temperatures ranging from 5-23ºC. The increase of thickness of water is shown as a function of increasing RH. Mg2+ mica has the highest water affinity among all the four mica surfaces.

Ion Adsorption and Hydration

Ion density and water density on mica surfaces in z-direction at 300K. Grey curves are water density plots. A snapshot of simulation box is given on the right.

The interplay of ion-water, ion-surface, and surface-water interactions affect ion adsorption and water structure.

Ice Nucleation via Seeding

Probable distribution of dipole orientations of water: blue curves are surfaces that promote ice nucleation; grey curves are surfaces that hinder ice nucleation.

Surface

Kao surface

Interfacial water structure in the metastable liquid state correlates with the propensity of observing ice nucleation at a given surface.

Monovalent ions mainly adsorb in the voids. Divalent ions have multiple adsorption states; both complete hydration and partial hydration is observed.

How do ions affect hydrogen bond network?

Hydrogen bond network in Mg2+-mica. Blue arrows indicate hydrogen bond between water molecules.