Secondary Ice Formation Process in Cirrus; A Simulation Study

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Introduction

Monitoring secondary ice formation in the atmosphere is experimentally challenging. Using molecular-scale simulations, evaluating these processes becomes possible. Experimental findings suggest surface abnormalities such as rough edges, cracks, and other defects are a more favorable site for nucleation than a surface without these imperfections. Modelling convex, concave, and flat ice surfaces allows for representation of all ice surfaces and their abnormalities. By also modelling different crystal planes, this accounts for all axes in which the water vapor may come into contact with the ice surface. The surface models are introduced to atmospheric conditions needed for secondary nucleation to occur. By observing how the three modeled surfaces interact with these conditions, it brings better understanding and predictability on the effect of surface characteristics on secondary ice formation.

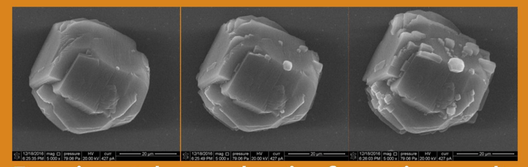
Methods

Two systems are modelled using a LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) script. Both scripts are written using atomic atom style (with no bonded interactions). It is modelled in this way because the bonds between Hydrogen and Oxygen are almost negligible in this case, allowing for a massive ease on computation. The first script models an ice surface designed to resemble experimental surfaces. There are two axes of ice Ih (hexagonal ice) modeled, the first is a crystal plane [1 1 0 0] (plane 3) and the other is a [0 0 0 1] (plane 4). The second script is written to mimic measured atmospheric conditions in cirrus clouds. Both scripts are then introduced to one another, allowing the ice surface to be exposed to atmospheric conditions. The output of these two scripts gives a “.dump” file which is evaluated by OVITO for data analysis. Built in OVITO modifications such as “CHILL+” helps gather the data and make it more observable.

Results

For a flat ice Ih surface being exposeto atmospheric conditions, a constant increase in ice Ih can be observed. The simulations ran for 3000 picoseconds. Plane 3's most notable growth was between 1000 and 1500 picoseconds while Plane 4 had an exponential growth throughout the simulation. The other notable ice that forms is interfacial ice which forms a layer on top of the ice sheet. This is to be expected as interfacial ice is dividing the different phases of water from vapor to Ice Ih. Interfacial ice had immediate and quick growth from 0 nanoseconds to 1500 picoseconds. It grew from 0 molecules to 1130 at the end with a peak of 1406 molecules at 2500 picoseconds. Ice Ic (cubic ice) is also formed very briefly. When the ice Ic is introduced to the ice Ih structure it undergoes a phase change to become ice Ih.

Fig. 4 - Experimental

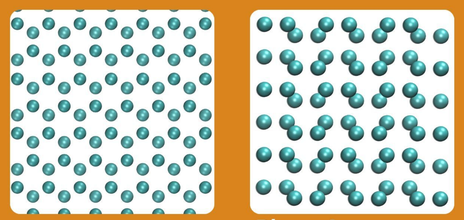


Experimental secondary ice formation results

Conclusion and Discussion

When a flat ice Ih surface comes into contact with atmospheric conditions, secondary ice formation mimics the initial surface properties, and the surface remains flat. Small imperfections and abnormalities can be observed in the surface over time. However, these defects are negligible due to the scale of the model. Growth of interfacial ice over the surface is expected due to water phases. Plane 3's ice growth was more abrupt than plane 4. It also ended with more ice surface area overall. The next steps is to model convex and concave ice surfaces and subject them to the same atmospheric conditions as the flat sheet.

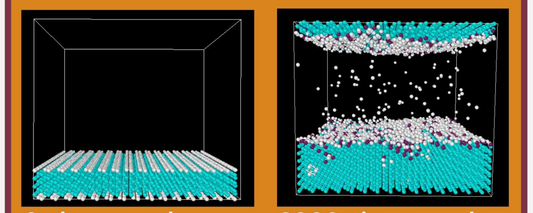
Fig. 1 - Crystal planes



Plane 3 Plane 4

Ice Ih structure with different crystal planes

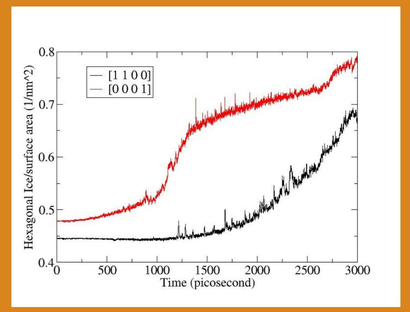
Fig. 2 - OVITO



0 picoseconds 3000 picoseconds

Flat ice Ih surface before and after deposition

Fig. 3 - Ice growth



Ice growth over time. Plane 3 and 4.

Acknowledgments and Refrences

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