Molecular Dynamics Determination of Edge-Sticking Parameters of Vicinal Ice Crystals

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Recommended Citation
Naatz, Sam, "Molecular Dynamics Determination of Edge-Sticking Parameters of Vicinal Ice Crystals" (2014). Summer Research. Paper 221.
http://soundideas.pugetsound.edu/summer_research/221
1. Introduction

Hexagonal ice crystals comprise a large percentage of cirrus clouds.1 Research shows that light scattering properties are influenced by roughness of crystals surfaces, which have climate impacts.2 However, the molecular mechanisms that give rise to surface roughness are not understood.

Molecular dynamics (MD) is a way to analyze such mechanisms by simulating ice crystal surface dynamics on a timescale of 100s nanoseconds. Previous MD work focused on “perfect” prismatic facets1 but it is known that growing cirrus ice crystals are vicinal i.e.: have steps. Theoretical work has indicated that molecular diffusion within the quasi-liquid layer (QLL) over and along these steps is key to the mechanisms growth and morphology.

This work examines diffusive dynamics of vicinal ice surfaces using MD. We focus primarily on the QLL, number of liquid-like molecules (N_{LL}), N_{LL} per area, and QLL thickness (d).

2. Objectives

Run simulations to analyze possible underlying theoretical mechanisms to crystal growth
• Do vicinal surfaces influence the QLL equilibrium?
• Is a discernable “edge” within the vicinal systems?
• Determine diffusion coefficients along and perpendicular (x and z axes) to edges

3. Computational Detail

Code made by Alicia Burns was used to rotate and cut originally “perfect” prismatic slab to create vicinal slab.

Two types of vicinal ice slabs (V_{1} and V_{2}) were constructed (2880 molecules) and annealed to seven target temperatures from 230 K to 287 K. After annealing, 100 ns production runs of each were used to create trajectories for analysis at each temperature.

The GROMACS utility 

\[
\mathbf{q} = \left[ (1/3) \sum_{j \neq i} \mathbf{r}_{ij} \cdot \mathbf{r}_{ij} \right]
\]

With q being the “tetrahedral order parameter". Where the \( \theta_{ij} \) angle is the angle created between oxygens i, j, and k within the crystal structure. The sums are for the four nearest neighboring oxygen atoms belonging to the central \( P \) water molecule. The tetrahedral order parameter uses a geometric orientation to characterize every molecule within the system. When q=1, the molecule is considered “ice-like”, any q<1, the molecule is considered “liquid-like”.2 The QLL thickness is estimated by the equation

\[
d = \frac{N_{LL}}{2ρN_{m}L_{x}L_{z}}
\]

Where N_{LL} is the number of liquid-like molecules, M is the molecular mass of water, ρ is the density of water, N_{m} is Avogadro’s number, and L_{x}, L_{z} are the dimensions of the ice slab.

4. Results

5. Conclusions

QLL is not significantly affected by vicinal slanting by statistical analysis

6. Future Directions

• Determine directional diffusivity in the x and z directions for current trajectories
• Use a perfectly flat prismatic slab with exact same dimensions to compare for perfect cross comparison
• Use large vicinal slabs with more distance between steps
• Use addition of 30+ molecules to determine timescale of equilibration of an additional “step”
• Determine the values of of the edge sticking parameters k +

Acknowledgements

Thanks to The University of Puget Sound. This work was supported by the National Science Foundation, grant CHE-1306366.