**An atoms-to-mesoscale approach to ice-vapor surface dynamics with a quasi-liquid interface**

Steven Neshyba1, Tia Böttger1, Rohan Crossland1, Spencer Racca-Gwozdzik1, Ella Slattery1, Maximilian Bloom, Noah Zimmer1, Penny M. Rowe2, and Jacob Price1

1University of Puget Sound, Tacoma Washington USA

2North West Research Association, Redmond Washington, USA

**Abstract**

*We explore the hypothesis that a key factor in determining the dynamics and morphology of faceted ice-vapor surfaces is the quasi-liquid layer that forms at this interface at temperatures above . We do so by modeling the ice surface as a system of reaction-diffusion equations in which the time scales of quasi-liquid freezing and melting, horizontal diffusion, and exchanges with the vapor phase are made explicit. Model parameterizations are informed by atomistic (molecular dynamics) simulations, mesoscale simulations of the vapor field around growing and ablating ice crystals, and quantitative ice surface morphologies derived from scanning electron microscope experiments. The outcome is a more unified, predictive, and experimentally grounded picture of the dynamics and morphology of faceted ice-vapor surfaces than has previously been presented.*

**Plain Language Summary**

This is a mathematical exploration of the texture of ice surfaces on a microscopic scale. The main hypothesis is that this texture is governed by the behavior of a thin layer of water, intermediate between ice and liquid, that is known to form at the ice-air interface. We carry out this exploration by constructing a set of mathematical relationships that, when solved on a computer, reveal how parts of this quasi-liquid layer migrate to other regions of the ice surface, freeze, or evaporate into the air. The form and parameters of these equations are informed by insights from images of ice surfaces from scanning electron microscope experiments, and molecular-level modeling. We believe the insights obtained from this effort will be useful not only from a fundamental perspective, but also practically, especially in connection to the role of ice clouds in Earth's climate system.

1. **Introduction**

Why we care about ice crystal morphology … the crystals that make up cirrus clouds modulate Earth’s climate by reflecting or scattering sunlight before it reaches Earth’s surface, but the extent to which they do that depends on the morphology of those crystals. Hexagonal prisms dominate, but there are lots of variations on that theme: long and thin hexagonal needles, short and wide plates, sometimes indented at the ends, or hollowed, or even dendritic forms, like snowflakes. Their surfaces can be smooth or rough on a scale that matters to light of comparable wavelength (Järvinen et al. 2023).

Numerous models of ice surface morphology and dynamics during vapor depositional growth have been presented. Harrington and Pokrifka (2021) provide an excellent review. Of these, models rooted in atomistic structure and processes are appealing because of the evident connection between molecular structure on the one hand, and high-resolution microscopic observations (such as scanning electron microscopy) on the other; a familiar example is that crystals of water ice are understood to owe their hexagonal shape to the hexagonal structure of the unit cell of an ice lattice. Molecular Dynamics studies have contributed greatly to this effort (see, e.g., (Llombart, Noya, and MacDowell 2020))

Of particular interest here is the Burton-Cabrera-Frank theory of crystal growth, also called classical nucleation theory, or CNT. CNT’s atomistic view of the process of crystal growth goes along the following lines: when a gas-phase molecule (e.g., a water molecule) encounters a crystalline surface, it initially becomes attached to that surface as an “admolecule.” Not yet part of the crystal’s lattice, this admolecule diffuses across the surface until it meets one of two fates: either it fills an unoccupied position in the crystal lattice (often visualized as a step between ledges), or else it returns the gas phase. New layer formation is governed by a 2D nucleation process in which the step free energy plays a crucial role (Kuroda and Lacmann 1982).

CNT has long framed how we think about ice crystal growth from the vapor phase, but it suffers from two drawbacks. First, it offers little guidance when it comes to describing the behavior of crystals placed in a vapor field that is *inhomogeneous* on a mesoscopic scale. To be specific, when a growing faceted ice crystal is situated in a supersaturated vapor field, it is easy to show that the surrounding water vapor concentration will be drawn down in such a way that facet intersections (i.e., crystal corners) will experience persistently higher vapor pressures than facet centers. CNT predicts that this would result in faster growth at those corners, leading ultimately to dendritic forms (e.g., snowflakes). An analogous circumstance arises when faceted crystals are situated in a subsaturated vapor field, in which case water vapor ablated from the surface distributes itself in such a way that crystal corners experience persistently *lower* vapor pressure compared to facet centers, which would lead to rounded crystal forms. However, under typical cirrus cloud conditions, it is known that hexagonal prisms resist both tendencies – that is, hexagonal faceting is resilient to imhomogeneities in the overlying vapor field. Classical nucleation theory has no satisfactory explanation for this resilience. (However, see Jayaprakash et al (1983)).

A second shortcoming of CNT is a lack of fealty to what is known about the molecular structure of the ice-vapor interface. When the temperature of ice rises above , both experiment and theoretical studies have shown that the ice/air interface is entirely covered by a quasi-liquid layer (QLL); molecular dynamics studies have shown that water molecule striking the surface are thermalized by the QLL efficiently and quickly (on a picosecond time scale) (Neshyba et al. 2009). On the other hand, recent experimental work has shown that there really are steps and ledges *underneath* the QLL, i.e., at the interface between the QLL and the underlying ice (Murata, Nagashima, and Sazaki 2019).

Bridging the gap between atomistic and mesoscale levels, therefore, calls for an approach that begins with the existence of a QLL (above ) in a way that preserves key parts of CNT as much as possible. We summarize this approach in the next two sections: In section 2 we review the qualitative features, key results, and limitations of a prior version of a quasi-liquid continuum model introduced by some of the authors (Neshyba et al. 2016, henceforth N2016). Section 3 presents a revised model that addresses these limitations. Section 4 discusses implications of these results in other contexts, including cirrus ice crystal morphologies and ideas from nonlinear dynamics, especially the properties of traveling waves of reaction-diffusion systems.

1. **Previous version of a Quasi-liquid continuum model (QLC-1)**

A Quasi-liquid-continuum model presented by some of the authors in N2016 takes the form of a reaction-diffusion model. Here we review qualitative features of this model, since many of those features carry over into the revised model.

The main features QLC-1 are summarized in Fig. 1. Ice surface dynamics are described in terms of two mesoscale variables, and , representing the total thickness of the ice surface, and its quasi-liquid part, respectively. As shown in the figure, is bounded by two extremes, namely a minimum corresponding to the equilibrium thickness of surface I, and a maximum corresponding to the equilibrium thickness of surface II. These two microsurfaces also possess different volatilities: surface I has lower volatility (i.e., lower chemical potential), while surface II has higher volatility (higher chemical potential). The difference in volatility between these two microsurfaces is specified it terms of a supersaturation difference, . (Evidence for the existence of these microstates, and their difference in volatility, emerges from molecular dynamics simulations described in N2016.)

QLC-1 prescribes the time evolution of and by a pair of reaction-diffusion equations that represent processes that influence and , namely: (i) Exchange (deposition and ablation) of QLL molecules with the vapor phase, (ii) Diffusion of QLL molecules across the ice surface, and (iii) Interconversion of QLL molecules to/from the underlying ice.

|  |
| --- |
|  |
| **Figure 1**. Visual representation of mesoscale variables , , and , and processes affecting them, in QLC-1 (as well as the present revision, QLC-2) model. Dashed arrows represent processes affecting how these variables evolve over time. |

A key feature of QLC-1 is that the overlying water vapor supersaturation is specified parametrically as a function of position along the facet surface, so that inhomogeneities in the overlying vapor field can be imposed. For example, consistent with the situation that facet corners of growing ice crystals experience higher vapor supersaturation (Berg 1938), a typical parameterization is parabolic,

(1)

where is the fractional reduction of supersaturation at facet centers relative to facet corners,

(2)

Negative values of in this formulation represent subsaturation conditions.

A typical trajectory result is shown in Fig. 2, where it is seen that new layers have formed preferentially at facet corners (consistent with the Bergian parameterization of the overlying water vapor field).

|  |
| --- |
|  |
|
| **Figure 2**. An ice surface covered by QLL, as simulated by QLM-2. |

The main insight afforded by QLC-1 is that it provides a mechanism by which faceted ice crystal growth can occur, summarized as follows (the reader is referred to N2016 for a more complete and quantitative version of these arguments).

1. Designating the horizontal distance between new layers and their predecessors as “” (see Fig. 2), we see that ; this is because new layers typically form at facet corners, where the water vapor concentration is highest, as described above.
2. Horizontal diffusion moves quasi-liquid away from surface II regions of the surface, toward surface I regions, because the former is thicker than the latter. The result is an overall increase in the average volatility of the surface, causing the surface as a whole to experience a net “diffusive slowdown” in its growth rate.
3. In regions where is small, QLL thickness gradients are large. In Fig. 2(b), for example, it is clear that the gradient in QLL thickness at I’ is greater than at I. It follows that, in a growing ice crystal, more diffusive slowdown occurs at facet corners.

In summary, a flat facet exposed to supersaturated vapor will initially experience higher growth rates at its corners, because of higher vapor concentration there, which leads to a higher step density (smaller ) there, hence a reduction in the growth rate at corners relative to facet centers. When these effects become balanced – which can (and does) occur as an emergent property of the equations of motion defining QLC-1 (and QLC-2, as we will show here), the result is equal growth rates across the entire facet. The resulting traveling wave would be interpreted at the mesoscale (e.g., in a high-resolution optical or scanning electron microscopy experiments) as faceted growth.

Our goal in the present communication is to generalize the above insight to a more diverse set of overlying vapor fields, and to narrow the number and range of parameters by applying physical constraints. To do so, we address a structural limitation in QLC-1 having to do with the time scale of quasi-liquid/ice equilibration dynamics shown in Fig. 1, and employ a nondimensionalization technique. These are described next.

1. **Revised version of a Quasi-liquid continuum model (QLC-2)**

The main structural limitation of QLC-1 is that the time scale of the interconversion of quasi-liquid and ice is fixed relative to the other two processes (deposition/ablation and quasi-liquid/ice equilibration). In real crystal facets, these time scales could vary from facet to facet, or as a function of temperature and vapor pressure, and therefore should therefore be adjustable quantities within the theory. QLC-2 corrects this limitation by replacing the quasi-liquid/ice equilibration term in QLC-1 with a term that explicitly takes into account that time scale. The result is

(3a)

(3b)

where is the time scale of quasi-liquid/ice equilibration. Other terms are identical (or nearly so) to those used in QLC-1, but for completeness we note them here:

1. represents surface diffusion of the QLL; the underlying ice is considered immobile on time scales considered here.
2. is the rate at which vapor-phase water molecules strike the quasi-liquid; it is assumed that these stick with 100% efficiency, and thermalize on a picosecond time scale (i.e., instantaneously within the time scales of a QLC-2 simulation).
3. prescribes the thickness of quasi-liquid when it is in equilibrium with the underlying ice, according to

(4)

This formulation ensures that the QLL thickness varies continuously from the thin microstate (“surface I”) with thickness , to the thick microstate (“surface II”) with thickness . (Note the connection to work of (Benet et al. 2019, Eq. 8), that also shows a sinusoidal dependence.)

1. The surface supersaturation at a given position, (see Eq. 3a), is a function of both the microstate and the water vapor concentration above the surface. To account for different volatilities of surfaces I and II, we use

(5)

where is the supersaturation relative to surface I (Eq. 1). With this definition, surface I will have , while surface II will have . In other words, this definition defines to be a measure of the additional volatility of surface II compared to that of surface II.

We will assume here that both (a scalar quantity) and are fixed parameters of a given solution. (Eq. 5 is at slight variance with, and simpler than, the corresponding expression in QLC-1.)

1. is a first-order relaxation constant describing the time scale at which quasi-liquid/ice equilibrium is achieved. With this revision, we are able to specify the rate of quasi-liquid/ice equilibration relative to processes (i) and (ii). Specifying a small value for , for example, would represent the idea that quasi-liquid/ice equilibration is fast compared to those processes, while large would mean the opposite.

A nondimensional form of QLC-2, using and , has the form

(6a)

(6b)

where . We see that this substitution has resulted in an effective diffusion coefficient equal to 1, and an effective quasi-liquid/ice equilibration time also equal to 1. The utility of this form is that it exposes redundancies in the parameterization. For example, since and appear only as a product, it is not necessary to explore dependence on these parameters separately.

1. **Methodology**

For the purpose of exploring solutions to the QLC-2 equations of motion, it is necessary to assign values of the parameters appearing in the foregoing. For simulations presented in this communication, we have chosen the baseline values

* and
* (the thickness of a single layer of ice) , to approximate the thickness of a prismatic facet bilayer
* (the distance from facet center to corner)
* (the ice-QLL equilibration time constant)
* (temperature)
* (the growth/ablation rate of the crystal)

While neither nor appears directly in the equations of motion, other parameters may be computed from them. The surface diffusion coefficient, , for example, can be based on a fit of diffusion data of (Price, Ide, and Arata 1999) to the form

(7)

with , . Di Prinzio et al (Di Prinzio et al. 2020) report a surface diffusion coefficient of at -5°C, which (using this value of ) corresponds to .

The water vapor deposition speed, , also depends on temperature, according to the Hertz-Knudsen formula,

(8)

where is water’s equilibrium vapor pressure, and is its molar mass.

There remains, therefore, specification of the baseline surface supersaturation, . For this purpose, we employ an iterative scheme involving vapor field simulations around a growing or ablating ice crystal, as follows: For a chosen growth rate, , a set of far-field supersaturation values () is specified. A vapor field calculation for each produces a corresponding profile, each of which is then given as input to a QLC-2 model run. The profile that yields a QLC-2 growth rate closest to is identified as the winner, and parameters and describing it are designated the baseline values. Details are given in Appendix 1.

Once we have determined these “baseline” parameters, we explore variations on that baseline by explicitly varying them independently, while recognizing interdependencies identified by the nondimensionalized form of the equations of motion (Eqs. 6a and 6b).

ODE … Runge-Kutta45 …

1. **Results from QLC-2 simulations**

Here we describe the results QLC-2 simulations, focusing on curvature of growing faceted surfaces (and hence the implied horizontal distance between adjacent ice layers, described above as “”), and a comparison of facet curvature under growth vs ablation conditions.

Figure 3 shows a modeled ice crystal surface subjected to three overlying vapor field profiles. All lead to steady-state solutions, but the shape of those solutions depends on the shape of the vapor profile:

* Scenario *“V-shaped supersaturated vapor field”*

A “V”-shaped supersaturated water vapor profile is the profile expected for growing, isolated cirrus ice crystals. After , an initially-flat ice surface converges to a steady state in which the surface is dominated by primarily surface I microstates, and is overall convex-shaped. Faceted growth is facilitated by smaller at facet boundaries, which causes a reduction in the growth rate, compensating for the higher supersaturation at facet boundaries.

* Scenario *“-shaped supersaturated vapor field”*

A “”-shaped supersaturated water vapor profile concentration profile is *not* expected for growing, isolated cirrus ice crystals, but it is plausible in SEM experiments when other crystals are nearby. After , an initially-flat ice surface also converges, also to a steady state in which the surface is dominated by primarily surface I microstates, but in this case the overall shape is concave. Faceted growth is facilitated by smaller at facet center, which causes a reduction in the growth rate, compensating for the higher supersaturation at facet center.

* Scenario *“-shaped subsaturated vapor field”*

A “”-shaped supersaturated water vapor profile concentration profile is expected for ablating isolated cirrus ice crystals. After , an initially-flat ice surface converges to a steady state in which the surface is dominated by primarily surface II microstates, and is overall concave-shaped. Faceted ablation is facilitated by smaller at facet boundaries, which causes a reduction in the ablation rate, compensating for the more extreme subsaturation at facet boundaries.

|  |  |  |
| --- | --- | --- |
| V-shaped supersaturated vapor field | -shaped supersaturated vapor field | -shaped subsaturated vapor field |
|  |  |  |
|  |  |  |
|  |  |  |
|  |  |  |
| **Figure 3**. Simulations of baseline scenarios (see Table 1). Top row: vapor supersaturation profiles; Second row from top: time evolution of the number of steps from facet centers to facet corners, beginning with a flat surface. Third row: total surface () and ice-only () thickness of the ice surface at simulation time; Bottom row: (i.e., ) at simulation time. | | |

A useful metric for describing the curvature of steady state profiles such as those appearing in Fig. 3 is the mean horizontal distance between successive molecular layers, defined as

(12)

|  |  |
| --- | --- |
| **Figure 4**. Mean horizontal layer separation, , as a function of … |  |

Lastly, we investigate the resilience of steady-state solutions to perturbations. The sequence of images in Fig. 5 begins with an initially-flat profile, which is then subjected to the following sequence:

1. From to , the surface is been exposed to the supersaturated water vapor curve shown in the inset located in the upper right part of the figure. By , the profile has evolved to the faceted, steady-state profile labeled “A”.
2. From to , a perturbation is introduced in the form of the subsaturated water vapor curve shown in the inset located in the middle-right part of the figure. During this time, the surface evolves into the highly perturbed state labeled “B”.
3. From to , the initial supersaturated water vapor regime is restored. During this time, the surface recovers its pre-perturbation faceted profile labeled “C”.

|  |
| --- |
|  |
| **Figure 5**. Examination of model facet resilience. Curves in the upper-left graph show timelines of that characterize the surface when subjected to the supersaturation curves shown in the upper-right insets, over the indicated time intervals. |

Conclusion … . Thus, we see that a key characteristic length predicted by QLC-2 depends on the square root of the surface diffusivity. This dependence is hallmark of Turing’s analysis of instability of reaction-diffusion systems leading to pattern formation. However, it should be borne in mind that the patterns of QLC-2 “steady states” are actually traveling-wave limit cycles, which are not considered in Turing’s analysis. Any such connection must overcome another hurdle as well, namely, that the depths of these characteristic distances are vastly different in QLC-2 compared to experiment: in the former it is a few monolayers, while in the latter it is thousands of monolayers.

In terms of facet resilience, we have seen that QLC-2 solutions and SEM-grown ice crystals both exhibit a propensity for perturbed states to recover when conditions favorable to faceting are restored.

1. **Summary and discussion**

The QLC-2 model presented here offers significant technical improvements over the QLC-1 model reported in N2016, in that its equations of motion embody a more faithful representation of ice/QLL freeze/melt equilibration, as indicated by Molecular Dynamics simulations. That connection, in turn, enables the theory to represent a more unified picture of ice surface dynamics than has previously been possible. The model predicts facet convexity and concavity, a pattern that is echoed in reconstructions of SEM-grown ice crystals. The model also provides a mechanism by which real ice crystals resist dendritic geometries when subjected to supersaturation conditions (i.e., faceted growth), and how they also resist rounding when subjected to subsaturation conditions (faceted ablation). It is, essentially, a theory of faceting that rests fundamentally on atomistic variations in the thickness and volatility of the quasi-liquid layer.

Qualitative implications of this work for cirrus cloud particles can be summarized as follows: As such particles fall through Earth’s atmosphere, such crystals will encounter increased pressure, hence smaller , but also increased temperatures (unless there is an atmospheric inversion), hence larger . When the effect of increased pressure dominates, QLC-2 predicts enhanced growth at facet corners, hence greater facet convexity, and therefore a greater propensity toward hollowed crystal structures. When the effect of increased temperature dominates, however, we can expect more regular hexagonal shapes. Although there is no single observational datum that would help us resolve these predictions, we can comment that in exceptionally cold regions (such as the Antarctic Plateau), or even in mid-latitudes where high-altitude cryo-capture of ice crystals on ground-launched balloons is possible, observations have shown that cirrus clouds are frequently hollowed, suggesting dominance of increased pressure distinctive (Magee et al. 2014, 2021; Walden, Warren, and Tuttle 2003).

We should note that the results presented here do not consider variations in parameters , and , because these values are highly uncertain; more detailed molecular dynamics calculations could provide plausible values, but those studies have not been reported. We can speculate that because different facet types (basal, prismatic, or pyramidal) have distinct underlying crystal cell structures, their quasi-liquid properties will also be Exploratory numerical studies varying the thickness of a single “layer” of ice has shown that a proportional increase in results. Preliminary numerical experiments varying and have shown that …

A separate speculation concerns the observation that the dependence of values exhibited by QLC-2 is the same as in Turing patterns. In one sense this should come as no surprise, since Turing’s theory, like QLC-2, is based on a reaction-diffusion equation. But there are also very big differences, including the fact that Turing’s analysis proceeds from an analysis of sensitivity to perturbations to an initially homogeneous distribution of chemical species, whereas the patterns in QLC-2 emerge as steady states of the equations of motion. The work of (Arioli and Koch 2015), on traveling-wave solutions of reaction-diffusion equations, is relevant here.

Finally, we note that the atoms-to-mesoscale approach represented in QLC-2 is not as fully integrated as we would like it to be … maybe some insight from Jake’s heterogeneous multiscale approach is the way forward on this (Shohet et al. 2020).

**Appendix 1 – Vapor field code**

Simulation of the water vapor partial pressure, , in the space surrounding a square-shaped crystal shown in Fig. A1(a), was achieved by integrating the two-dimensional diffusion equation

(A1)

where is the diffusion coefficient of water vapor through air, which is computed by (see Air-Diffusion Coefficients of Gases in Excess of Air),

(A2)

Equation A1 is solved subject to Neumann boundary conditions that represent depletion of water vapor in the layer adjacent to the crystal surface due to crystal growth. This rate of depletion is given by

(A3)

where

* + , the specified growth rate of the ice surface;
  + , the mass density of ice; and
  + , the molar mass of water

Dirichlet conditions representing the far-field vapor concentration (), are imposed at the outside boundary of the simulation space. Integration over time was performed using Euler’s method, parameters for which are given in Table A1.

|  |  |
| --- | --- |
| **Table A1. Parameters for simulation of the vapor field around a growing, square-shaped ice crystal** | |
| Simulation space dimensions |  |
| Time step for integration |  |
| Time interval for integration |  |
| Spatial discretization |  |
| Diffusion coefficient at , |  |
| Ambient temperature |  |
| Ambient pressure |  |
| Diffusion Temperature-correction exponent |  |
| Diffusion coefficient under ambient conditions |  |
| Far-field water vapor partial pressure |  |
| Far-field water vapor supersaturation |  |
| Far-field distance from the origin |  |
| Mass density of ice |  |
| Growth rate of ice surface |  |

The resulting vapor concentration contours shown in Fig. A1(a) are seen to decrease with proximity to the crystal, as expected since the growing crystal is drawing water vapor out of the surrounding air. This reduction is greater at facet center compared to facet corners, in a roughly parabolic fashion, as shown in the profile in Fig. A1(b).

|  |  |
| --- | --- |
| (a) | (b) |
|  |  |
| **Figure A1**. (a) Simulation of vapor partial pressures, , in units , around a growing ice crystal. The black-outlined box at the center indicates the surface of the crystal, in this case spanning . Contours outside the crystal show values of at steady state. Dirichlet conditions fix a partial pressure of at the far-field distance of , while Neumann conditions representing ice growth are imposed at the ice surface (see text). (b) along the surface of the crystal. | |

Supersaturation values are computed from these values using

(A4)

These simulations are then used to obtain parameterizations for QLC-2 by the following steps:

1. , the growth rate of the ice surface, is obtained iteratively, as follows:
   1. A Vapor Field simulation takes growth rate of the ice surface () as an input, along with , , , and , and predicts and .
   2. A QLC-2 simulation takes and as inputs, along with , , , and , and predicts a new growth rate of the ice surface ().
   3. These steps are repeated until and agree within some tolerance level.

**Appendix 2 – ESEM/GNBF retrieval**

Here is a summary of key equations and constraints in the ESEM/GNBF retrieval …

**Appendix 3 – Numerical considerations**

Python, accelerated with Numby. Code and data are available on Github.

References:

Anon. n.d. “Air - Diffusion Coefficients of Gases in Excess of Air.” Retrieved February 4, 2024 (https://www.engineeringtoolbox.com/air-diffusion-coefficient-gas-mixture-temperature-d\_2010.html).

Arioli, Gianni, and Hans Koch. 2015. “Existence and Stability of Traveling Pulse Solutions of the FitzHugh–Nagumo Equation.” *Nonlinear Analysis: Theory, Methods & Applications* 113:51–70. doi: 10.1016/j.na.2014.09.023.

Benet, Jorge, Pablo Llombart, Eduardo Sanz, and Luis G. MacDowell. 2019. “Structure and Fluctuations of the Premelted Liquid Film of Ice at the Triple Point.” *Molecular Physics* 117(20):2846–64. doi: 10.1080/00268976.2019.1583388.

Berg, W. F. 1938. “Crystal Growth from Solutions.” *Proceedings of the Royal Society of London. Series A - Mathematical and Physical Sciences* 164(916):79–95. doi: 10.1098/rspa.1938.0006.

Di Prinzio, Carlos Leonardo, Damian Stoler Flores, Guillermo Gabriel Aguirre Varela, and Esteban Druetta. 2020. “Superficial Self-Diffusion Coefficient in Ih-ICE.” doi: 10.5817/CPR2020-2-12.

Harrington, Jerry Y., and Gwenore F. Pokrifka. 2021. “Approximate Models for Lateral Growth on Ice Crystal Surfaces during Vapor Depositional Growth.” *Journal of the Atmospheric Sciences* 78(3):967–81. doi: 10.1175/JAS-D-20-0228.1.

Järvinen, Emma, Bastiaan van Diedenhoven, Nathan Magee, Steven Neshyba, Martin Schnaiter, Guanglang Xu, Olivier Jourdan, David Delene, Fritz Waitz, Simone Lolli, and Seiji Kato. 2023. “Ice Crystal Complexity and Link to the Cirrus Cloud Radiative Effect.” Pp. 47–85 in *Clouds and Their Climatic Impacts*. American Geophysical Union (AGU).

Jayaprakash, C., W. F. Saam, and S. Teitel. 1983. “Roughening and Facet Formation in Crystals.” *Physical Review Letters* 50(25):2017–20. doi: 10.1103/PhysRevLett.50.2017.

Kuroda, T., and R. Lacmann. 1982. “Growth Kinetics of Ice from the Vapour Phase and Its Growth Forms.” *Journal of Crystal Growth* 56(1):189–205. doi: 10.1016/0022-0248(82)90028-8.

Llombart, Pablo, E. Noya, and Luis MacDowell. 2020. “Surface Phase Transitions and Crystal Habits of Ice in the Atmosphere.” *Science Advances* 6:eaay9322. doi: 10.1126/sciadv.aay9322.

Magee, N. B., A. Miller, M. Amaral, and A. Cumiskey. 2014. “Mesoscopic Surface Roughness of Ice Crystals Pervasive across a Wide Range of Ice Crystal Conditions.” *Atmospheric Chemistry and Physics* 14(22):12357–71. doi: 10.5194/acp-14-12357-2014.

Magee, Nathan, Katie Boaggio, Samantha Staskiewicz, Aaron Lynn, Xuanyi Zhao, Nicholas Tusay, Terance Schuh, Manisha Bandamede, Lucas Bancroft, David Connelly, Kevin Hurler, Bryan Miner, and Elissa Khoudary. 2021. “Captured Cirrus Ice Particles in High Definition.” *Atmospheric Chemistry and Physics* 21(9):7171–85. doi: 10.5194/acp-21-7171-2021.

Murata, Ken-ichiro, Ken Nagashima, and Gen Sazaki. 2019. “How Do Ice Crystals Grow inside Quasiliquid Layers?” *Physical Review Letters* 122(2):026102. doi: 10.1103/PhysRevLett.122.026102.

Neshyba, Steven, Jonathan Adams, Kelsey Reed, Penny M. Rowe, and Ivan Gladich. 2016. “A Quasi-Liquid Mediated Continuum Model of Faceted Ice Dynamics.” *Journal of Geophysical Research: Atmospheres* 121(23):14,035-14,055. doi: https://doi.org/10.1002/2016JD025458.

Neshyba, Steven, Erin Nugent, Martina Roeselová, and Pavel Jungwirth. 2009. “Molecular Dynamics Study of Ice−Vapor Interactions via the Quasi-Liquid Layer.” *The Journal of Physical Chemistry C* 113(11):4597–4604. doi: 10.1021/jp810589a.

Price, William S., Hiroyuki Ide, and Yoji Arata. 1999. “Self-Diffusion of Supercooled Water to 238 K Using PGSE NMR Diffusion Measurements.” *The Journal of Physical Chemistry A* 103(4):448–50. doi: 10.1021/jp9839044.

Shohet, Gil, Jacob Price, Jeffrey Haack, Mathieu Marciante, and Michael S. Murillo. 2020. “Heterogeneous Multiscale Method for High Energy-Density Matter: Connecting Kinetic Theory and Molecular Dynamics.” *Journal of Computational Physics: X* 8:100070. doi: 10.1016/j.jcpx.2020.100070.

Walden, Von P., Stephen G. Warren, and Elizabeth Tuttle. 2003. “Atmospheric Ice Crystals over the Antarctic Plateau in Winter.” *Journal of Applied Meteorology and Climatology* 42(10):1391–1405. doi: 10.1175/1520-0450(2003)042<1391:AICOTA>2.0.CO;2.