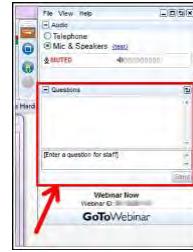




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7

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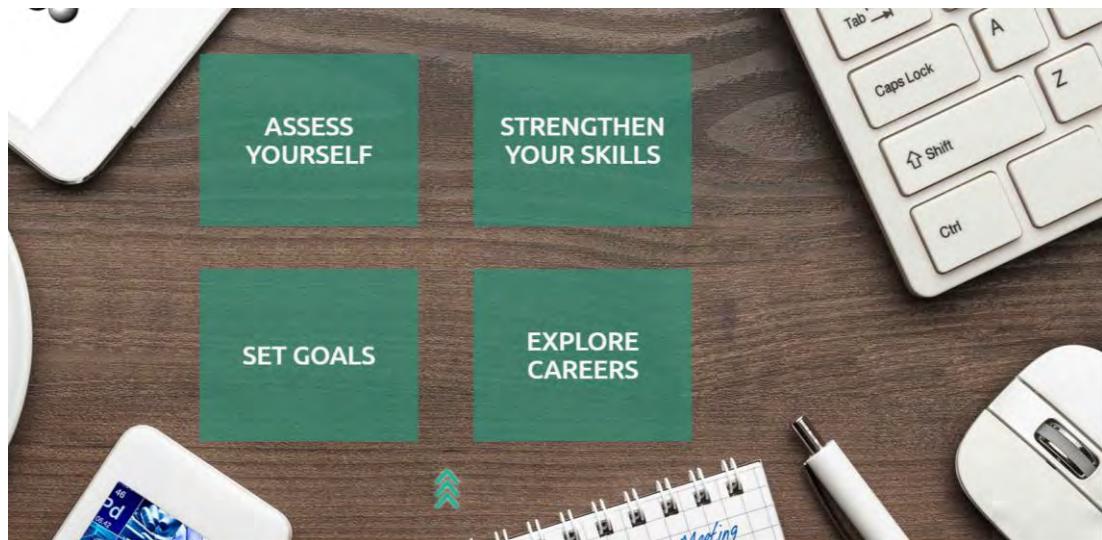


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<https://www.acs.org/content/acs/en/acs-webinars/technology-innovation/microtubule-targeting-agents.html>

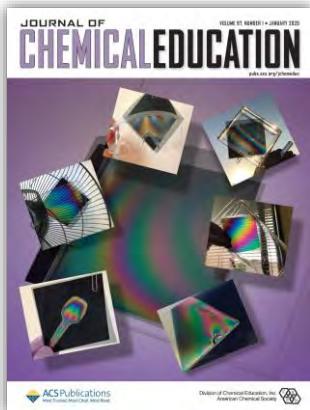
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<https://pubs.acs.org/journal/iceda8>

<http://divched.org> (NEW Website coming this March!)

11

THE SECRET LIVES OF SNOWFLAKES

Peculiarities in the Molecular Dynamics of Ice Crystal Growth

ACS Chemistry for Life®

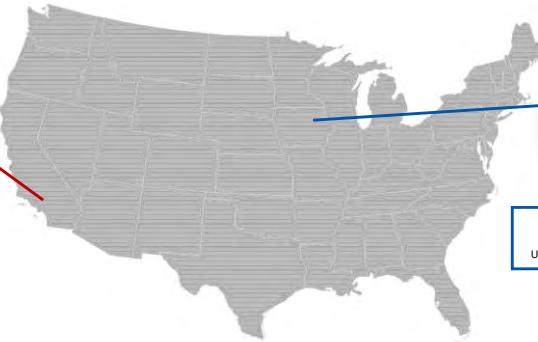
THIS ACS WEBINAR WILL BEGIN SHORTLY...

12

The Secret Lives of Snowflakes: Peculiarities in the Molecular Dynamics of Ice Crystal Growth



Kenneth Libbrecht
Professor of Physics, California Institute of Technology and snowcrystal author

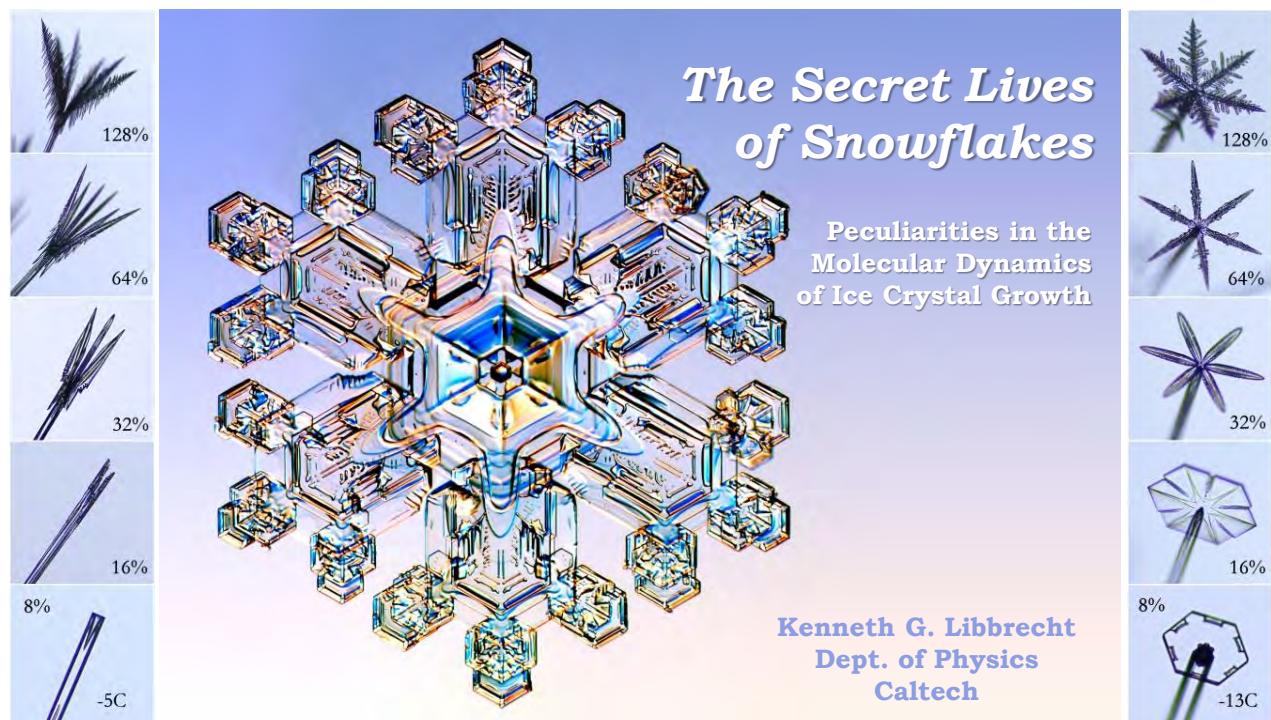


Dawn Del Carlo
Associate Professor of Chemistry Education, University of Northern Iowa and Chair, ACS CHED

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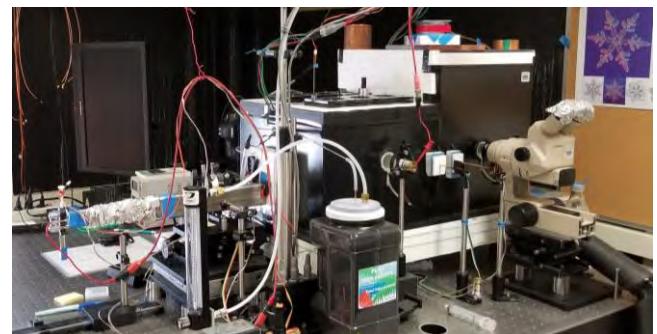
A laboratory “Snowflake on a Stick”



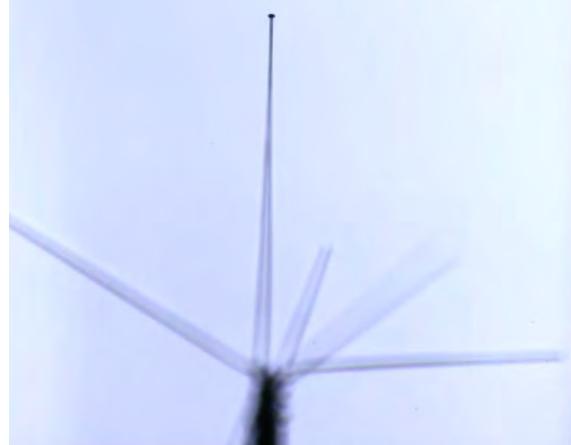
Environment:
Fixed temperature – $T < 0$ C
Fixed supersaturation – $\sigma > 0$
(RH > 100%)
In air at 1 atm

Add seed crystal
Thin ice needle
 ~ 2 mm long, ~ 5 μm diam

This example:
 $T = -15$ C, $\sigma = 16\%$
then 64%



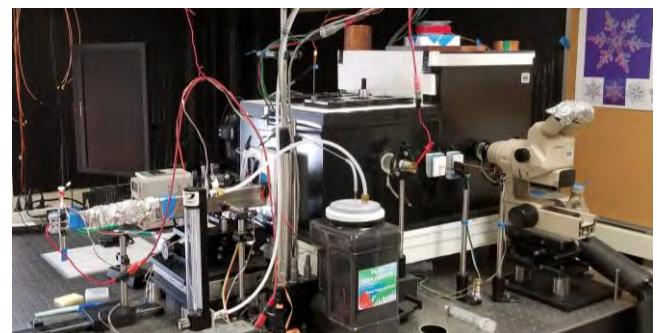
A laboratory “Snowflake on a Stick”



Environment:
Fixed temperature – $T < 0$ C
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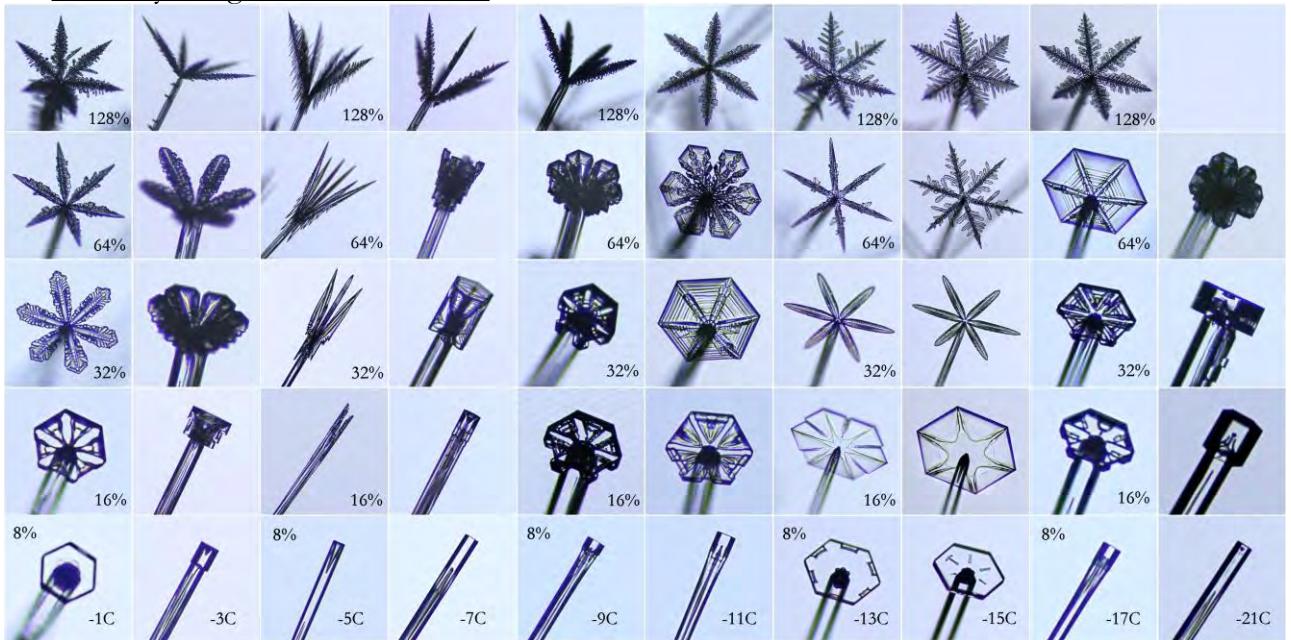
Snow crystals grown on ice needles



Unusual behavior as function of temperature

All single crystals; all grown at constant conditions

Snow crystals grown on ice needles



What is the underlying physics? Can make computer models?

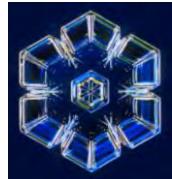
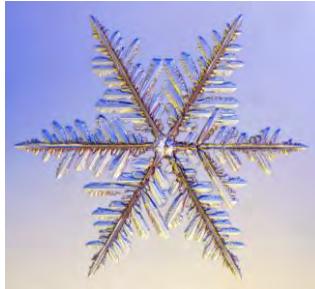
Can find these in nature also...



Natural Snow Crystals...

Stellar Crystals, form at -15C

(a primary characteristic: thin and flat)



22

Audience Survey Question

ANSWER THE QUESTION ON BLUE SCREEN IN ONE MOMENT



How large are typical stellar snow crystals in nature?

- About 0.1 millimeters from tip to tip
- About 0.3 millimeters
- About 1 millimeter
- About 3 millimeters
- About 10 millimeters



* If your answer differs greatly from the choices above tell us in the chat!

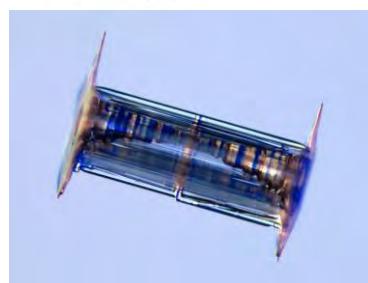
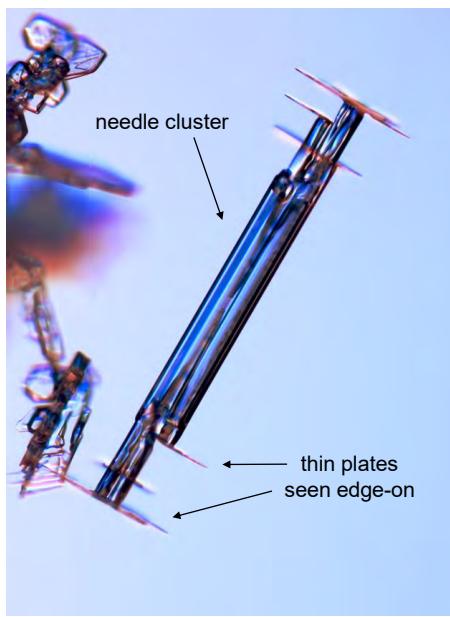


Natural Snow Crystals...
Size comparisons

Largest snow crystal
ever photographed,
10 mm tip-to-tip

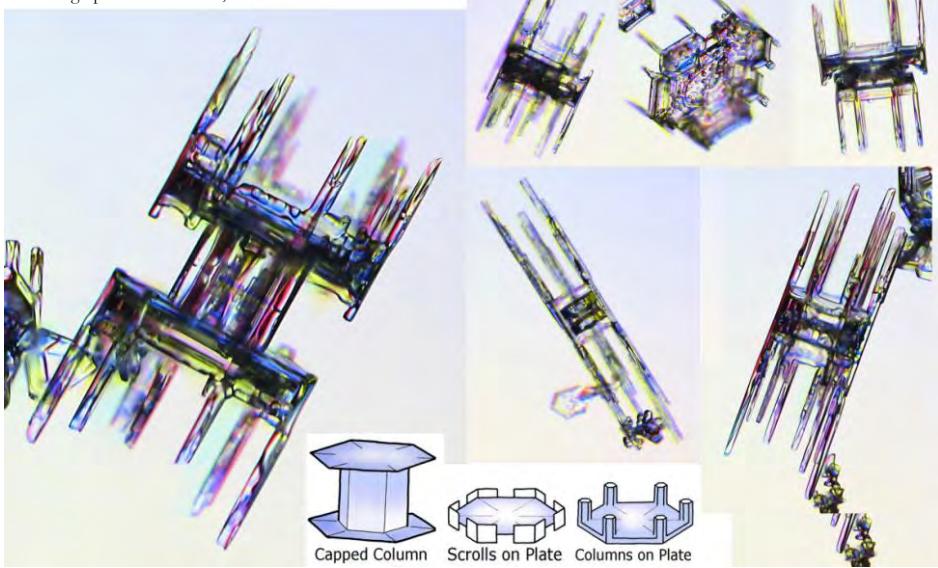


Natural Snow Crystals...
Capped Columns

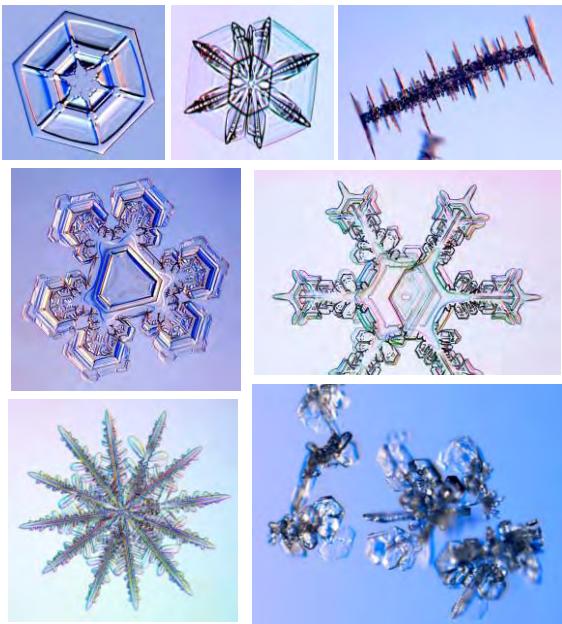


Some especially odd examples:
Capped columns with scrolls and columns

Photographed in Fairbanks, Alaska



A Menagerie of Natural Snow Crystals...



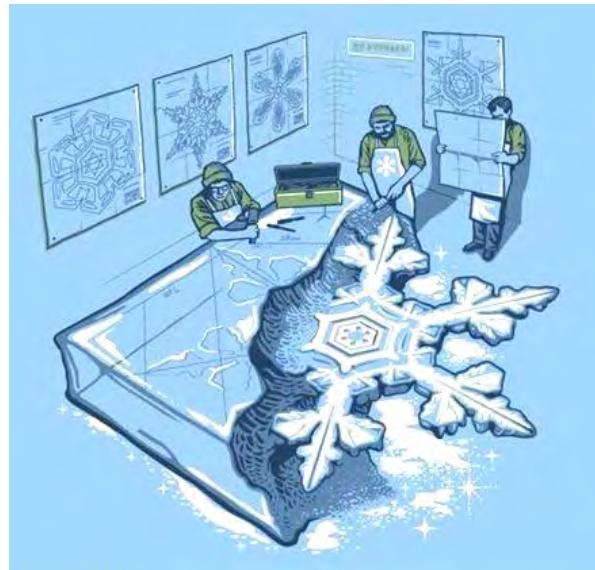
Simple Prisms	Solid Columns	Sheaths	Scrolls on Plates	Triangular Forms
Hexagonal Plates	Hollow Columns	Cups	Columns on Plates	12-branched Stars
Stellar Plates	Bullet Rosettes	Capped Columns	Split Plates & Stars	Radiating Plates
Sectored Plates	Isolated Bullets	Multi-Capped Columns	Skeletal Forms	Radiating Dendrites
Simple Stars	Simple Needles	Capped Bullets	Twin Columns	Irregulars
Stellar Dendrites	Needle Clusters	Double Plates	Arrowhead Twins	Rimed
Fernlike Stellar Dendrites	Crossed Needles	Hollow Plates	Crossed Plates	Graupel



from Ken Libbrecht's Field Guide to Snowflakes

What is the underlying physics?

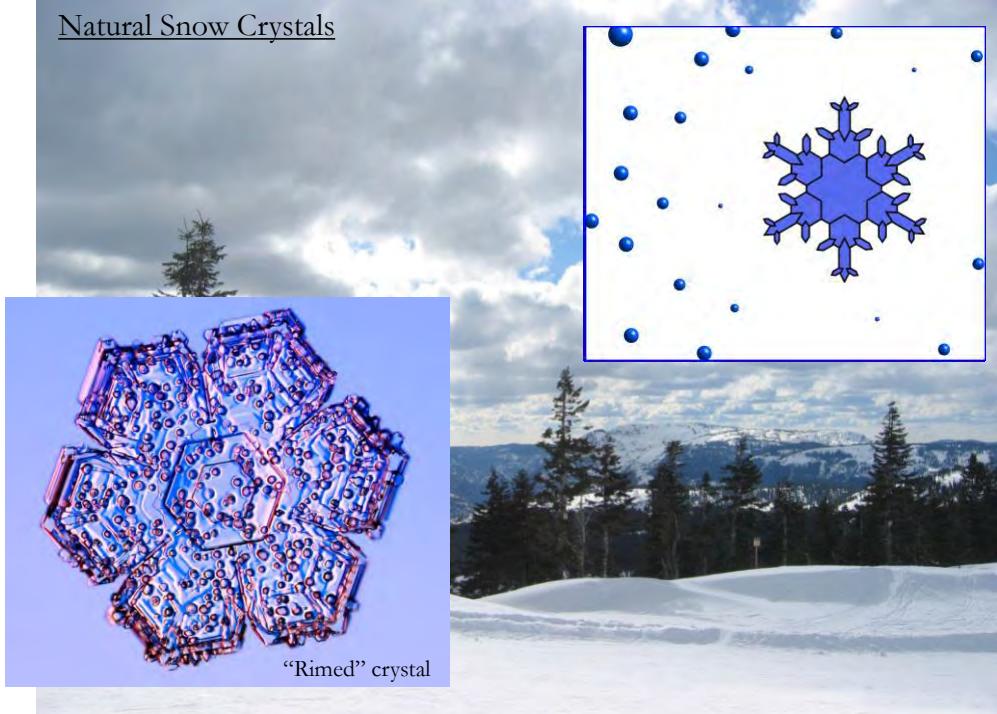
The wrong way to make a snowflake

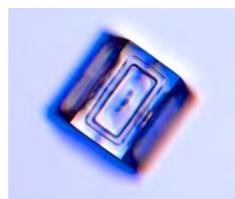


Christopher Buchholz

Nature makes things
using self-assembly...

Natural Snow Crystals

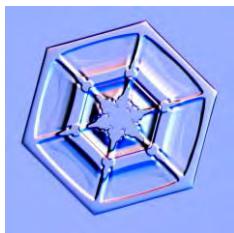
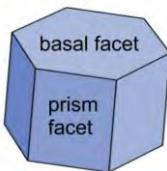
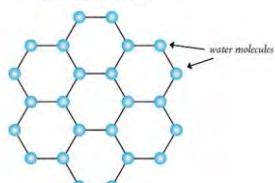




Snowflake Physics I - Faceting

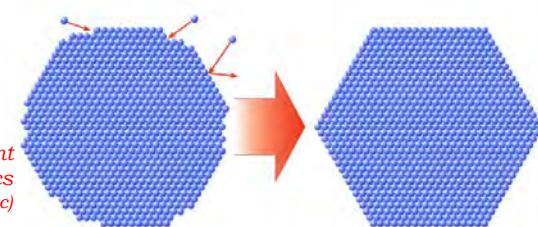
Structure of the Ice Crystal → Facets

AN ICE CRYSTAL

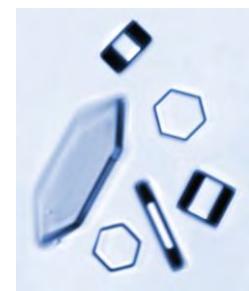


*Attachment Kinetics
(highly anisotropic)*

(Surface energy
not very important;
nearly isotropic)

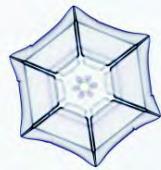


*Faceting is how the geometry of the water molecule
is transferred to the geometry of a crystal.*



Tiny,
laboratory
grown
snow
crystals
~0.1 mm

→ no 4-, 5-, 7-, 8-sided snow crystals!

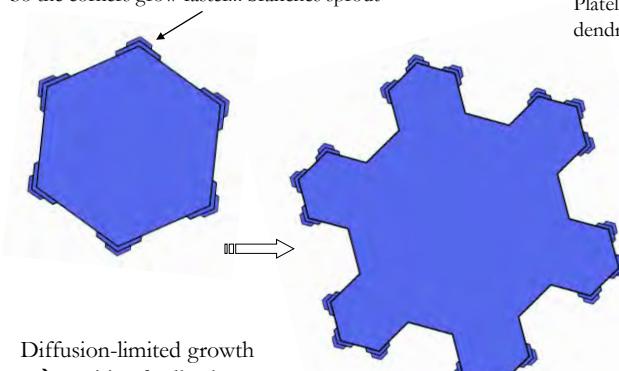


Snowflake Physics II – The Branching Instability

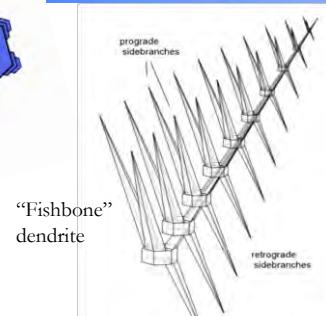
(a.k.a. the Mullins-Sekerka instability; 1963)

Particle diffusion through air is key (heat diffusion less important)

The six corners stick out farther into the humid air
So the corners grow faster... branches sprout



Platelike dendrite



Snowflake Physics III - Complexity and Symmetry

(an explanation of the “No-Two-Alike” conjecture)

- Nucleation of ice particle

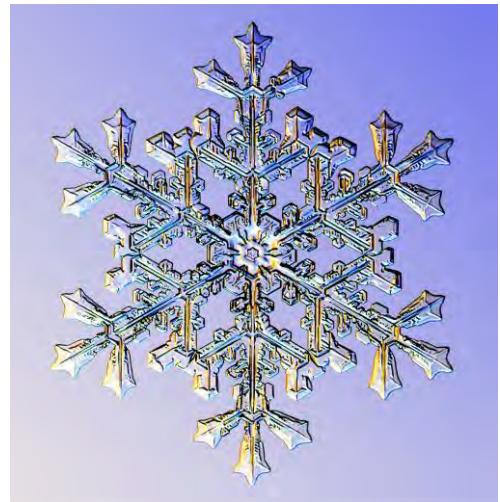
Grows to hexagonal prism, since smooth facets grow most slowly (stellar snow crystal)

Simple plate unstable as crystal grows larger ... corners sprout arms

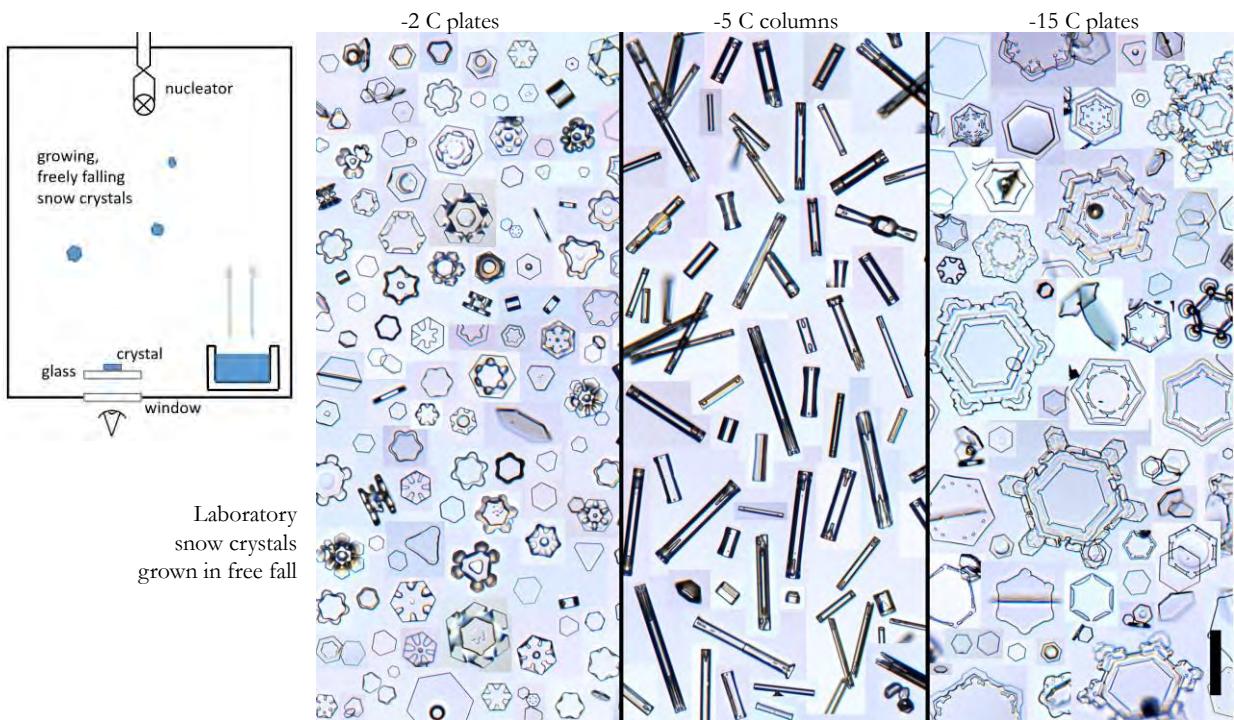
Crystal moves to different temperature ... plates grow on arms

Crystal moves through *many different temperatures, humidities ...* each change causes new growth behavior on arms

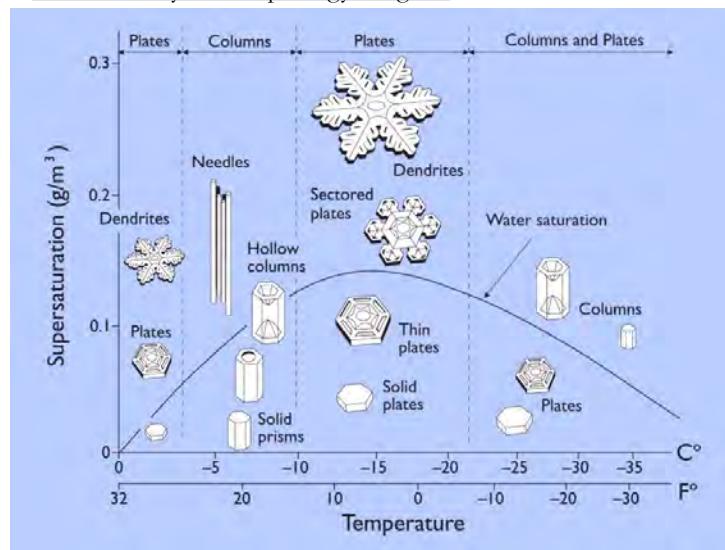
Complex history → Complex crystal shape, faceted & branched
 Each arm experiences same history → Symmetry
 No two paths are the same → No two alike
All because growth sensitive to temperature, humidity



How explain morphology versus temperature and supersaturation?



The Snow Crystal Morphology Diagram A “Rosetta Stone” for Snow Crystals



An unsolved puzzle for 65 years... a purely empirical result

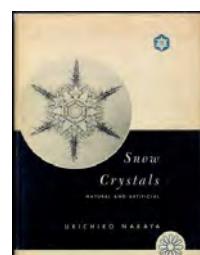
Solved at last?

KGL, arXiv:1910.09067
arXiv:1910.06389

Attachment kinetics is key → Examine facet growth



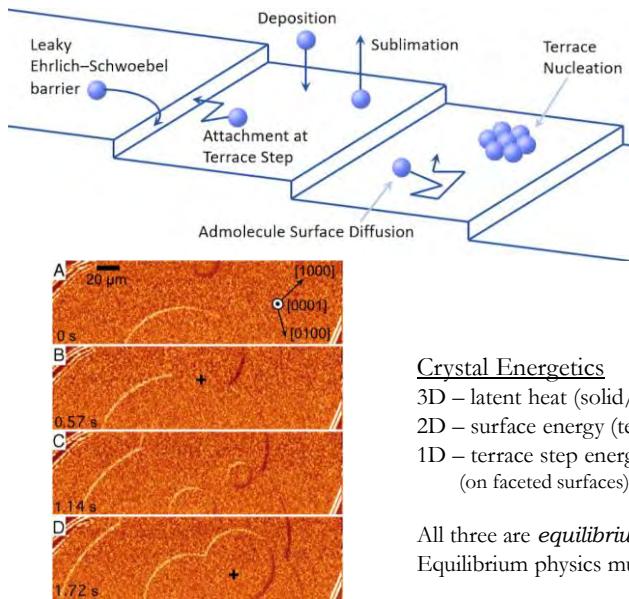
Ukichiro Nakaya
~1930s
Hokkaido University



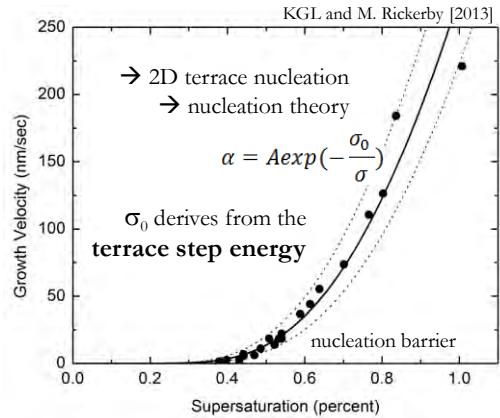
Snow Crystals, Natural and Artificial, 1954



Precision Measurements of Facet growth & Step energies



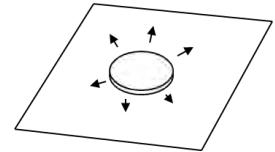
Imaging Ice Terraces, Sazaki et al, 2010



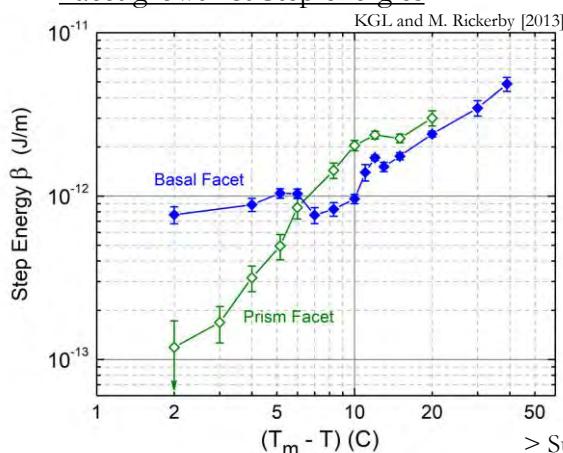
Crystal Energetics

- 3D – latent heat (solid/vapor) ... energy to vaporize crystal
- 2D – surface energy (tension) ... energy to break bonds and create surface
- 1D – terrace step energy ... energy to split island terrace
(on faceted surfaces)

All three are *equilibrium* material properties
Equilibrium physics much easier than dynamics

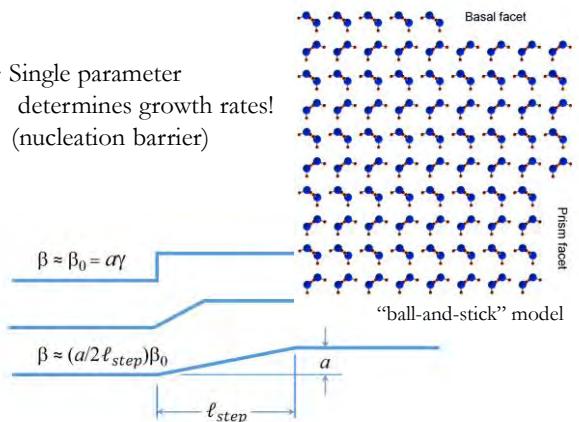


Facet growth & Step energies



- QM → molecules → interactions
- MD simulations → step energies
- comparison with measurements

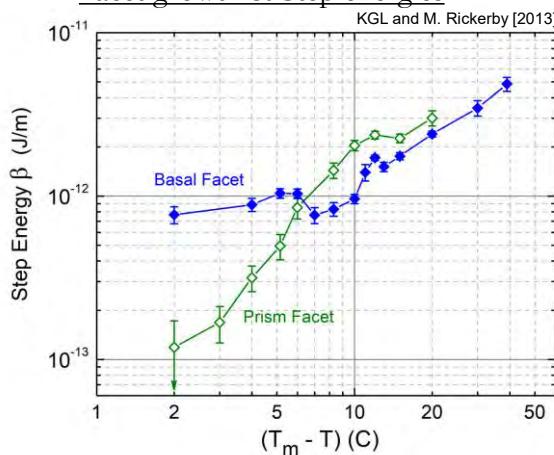
> Single parameter
determines growth rates!
(nucleation barrier)



- > Surface relaxation lowers step energy
- > Calculate from molecular-dynamics (MD) simulations?
In principle, yes! ... equilibrium quantity
Already have good ice/water MD models

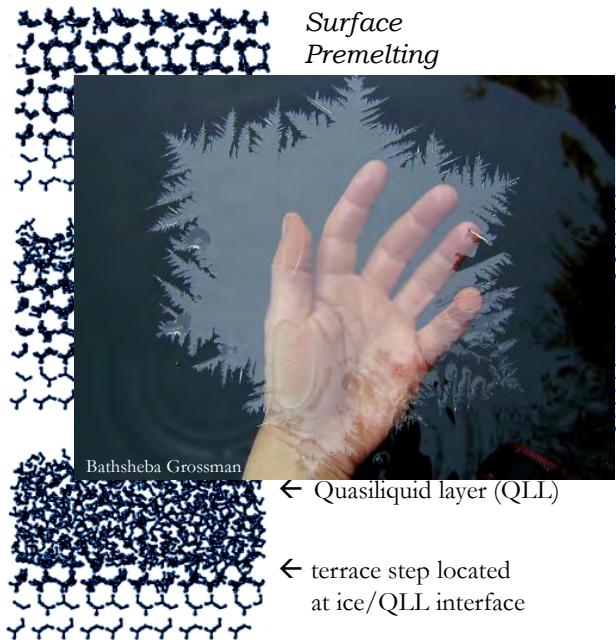
> T. Frolov and M. Asta, J. Chem. Phys. 137, 214108, 2012 (silicon)
> Jorge Benet et al., Molecular Phys. 0026-8978, 2019 (ice)

Facet growth & Step energies



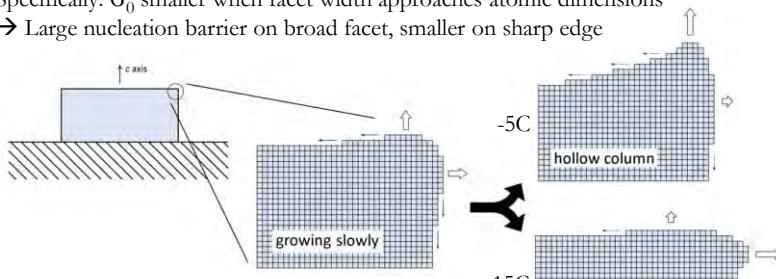
QM → molecules → interactions
→ MD simulations → step energies
→ comparison with measurements

Still need more physics to explain the morphology diagram ...



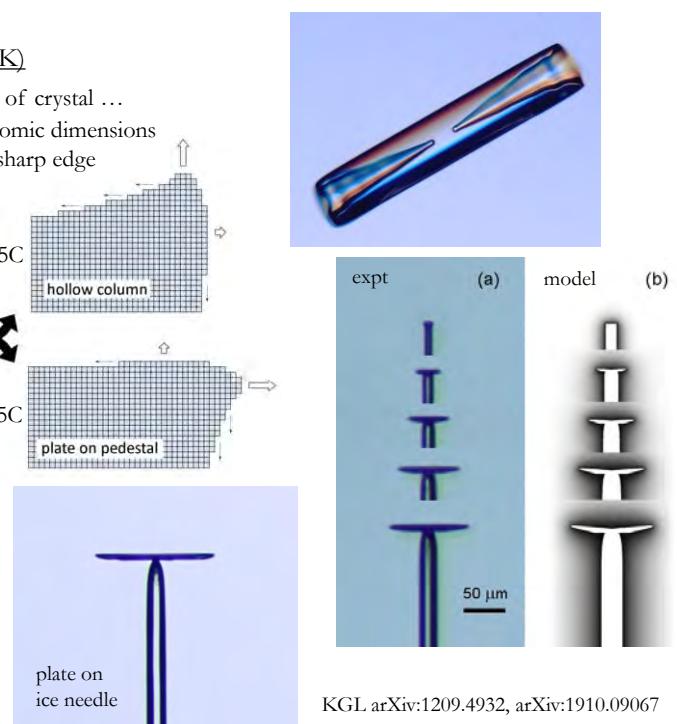
Structure Dependent Attachment Kinetics (SDAK)

Attachment kinetics depends on *mesoscopic* structure of crystal ...
Specifically: σ_0 smaller when facet width approaches atomic dimensions
→ Large nucleation barrier on broad facet, smaller on sharp edge

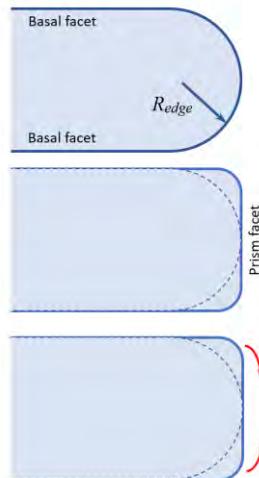


Caused by surface diffusion onto terraces
... enhanced by surface premelting
→ an *edge-sharpening SDAK instability*
→ promotes the formation of
thin plates & hollow columns

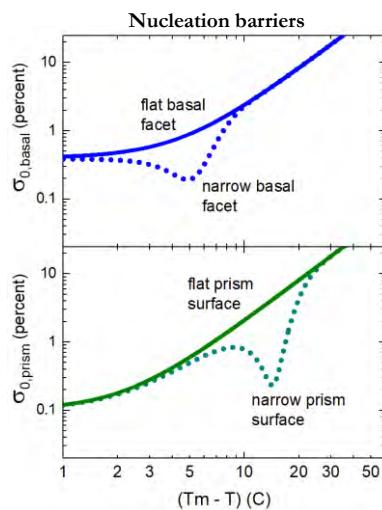
An enhanced diffusion-limited growth model
→ changes *anisotropy* of attachment kinetics
SDAK instability helps explain
abrupt transitions in the morphology diagram



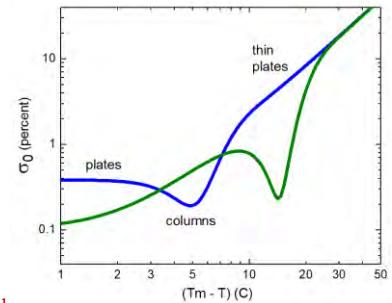
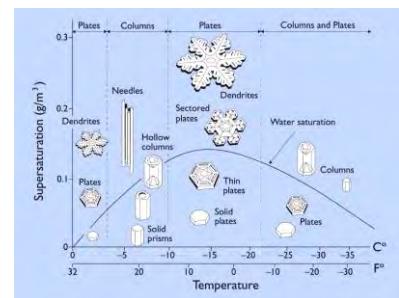
Structure Dependent Attachment Kinetics (SDAK)



Surface diffusion
from corners to facets
enhanced by surface premelting



→ A Comprehensive, Quantitative Model



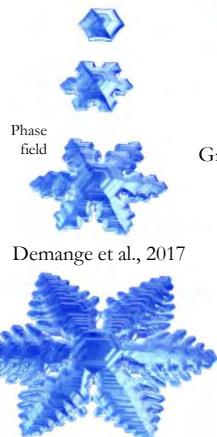
A 65-year-old puzzle...solved at last? arXiv:1910.09067
Have enough now to start making 3D models

3D Numerical Modeling – lots of recent progress

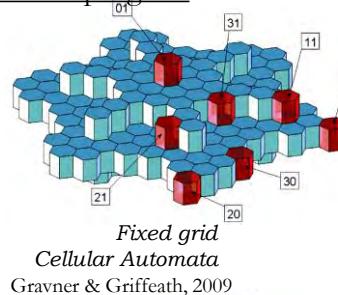
Solving diffusion equation easy
Surface boundary conditions tough
Facets → cusp-like behavior
No branched+faceted structures until ~2008



Barrett, Gärcke,
& Nürnberg, 2012



Demange et al., 2017



Fixed grid
Cellular Automata
Gravner & Griffeath, 2009



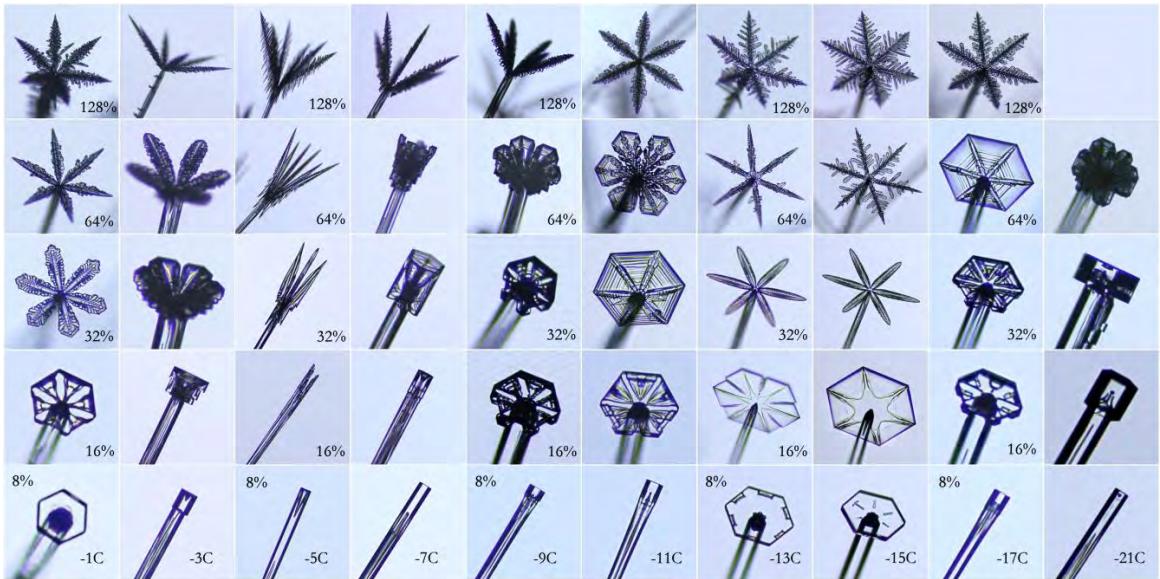
3D CA Model by
David Griffeath
& Janko Gravner
Rendered by
Antoine Clappier



Kelly & Boyer, 2014

So far, morphology demonstrations only ... quantitative models possible

Creating a comprehensive model of snow crystal growth



QM → atoms & molecules → interactions → MD simulations → step energies, surface diffusion, premelting
 → full attachment kinetics (SDAK) → numerical modeling → 3D structures, growth rates → experiments
 ...???

Rainbow Physics

Aristotle (Greece, ~350 BC)
 Seneca the Younger (Rome, ~65 AD) – droplets
 Shen Kuo (China, ~1060) – droplet theory
 Qutb al-Din al-Shirazi (Persia, ~1260) – droplet reflections
 Kamāl al-Dīn al-Fārisī (Persia, ~1300) – sphere experiments
 Roger Bacon (England, 1268) – droplet colors
 Theodoric of Freiberg (Germany, 1307) – primary, secondary bows
 Willebrord Snell (Netherlands, 1621) – refraction
 René Descartes (France, 1637) – reflection+refraction, caustics
 Isaac Newton (England, 1672) – dispersion → colors
 Thomas Young (England, 1803) – diffraction → supernumerary rainbows
 George Biddell Airy (England, ~1820) – refraction theory
 Gustav Mie (Germany, 1908) – scattering theory



Steve Nelson (Fayfoto, Boston MA)

Snow crystal formation: A case study of the molecular physics of crystal growth



Why Ice?

- > Monomolecular system
- > Well characterized material
- > Molecular dynamics simulations well developed
- > Growth from vapor → temperature & supersaturation
- > Rich phenomenology, largely unsolved
- > Inexpensive experiments; no safety issues
- > A self-contained molecular physics puzzle

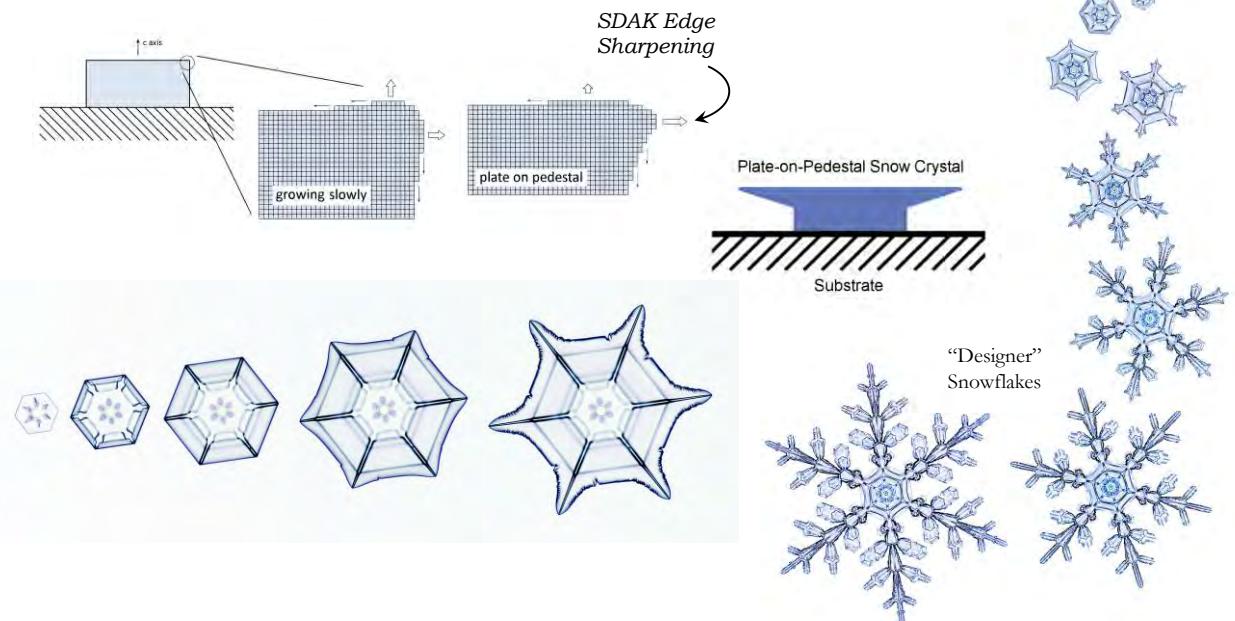
But ... no (direct) applications ... *zero tax dollars*

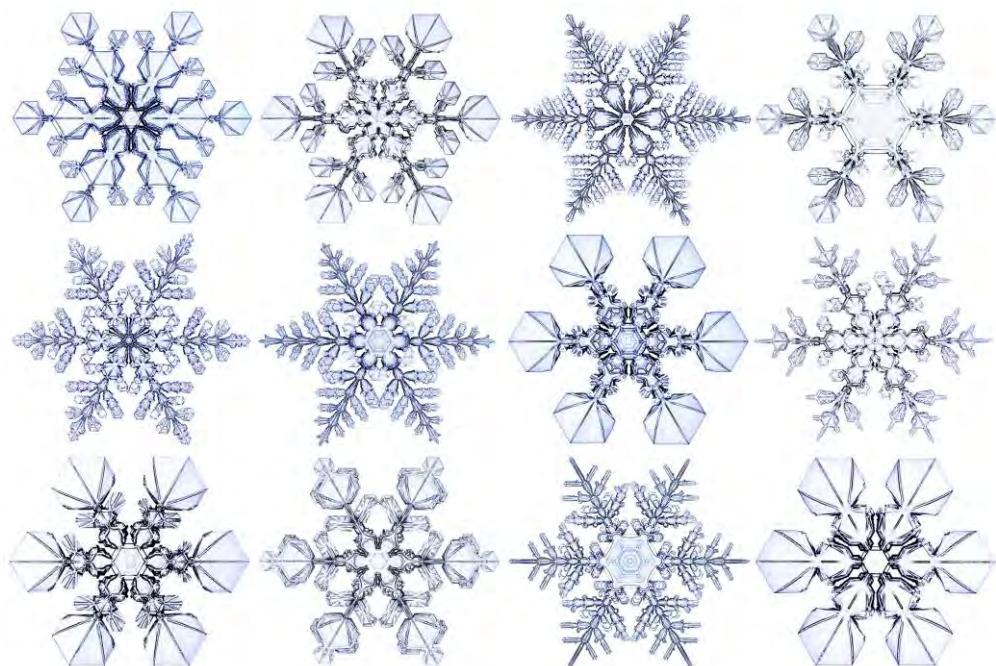
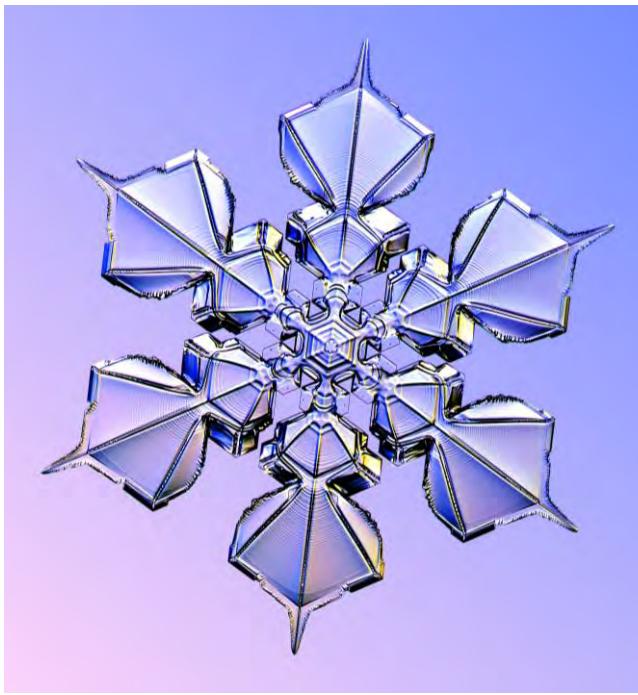
overarching goal is to understand crystal growth



book royalties pay the bills...

Snowflake Engineering – Plate-on-Pedestal Snow Crystals







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Audience Survey Question

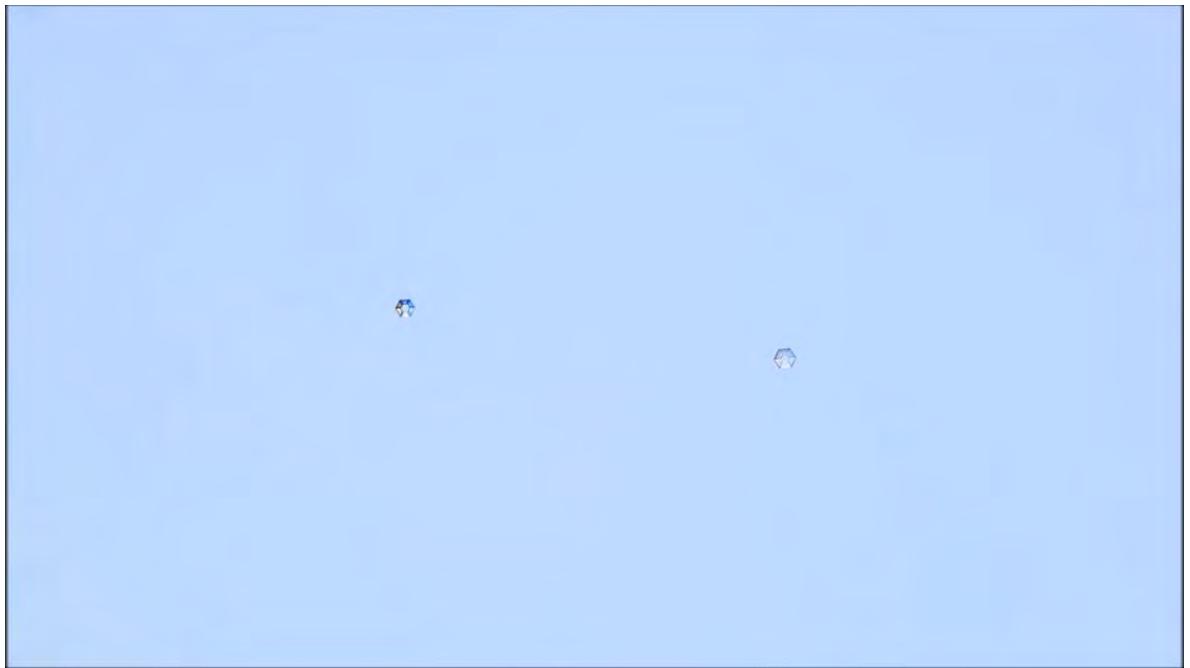
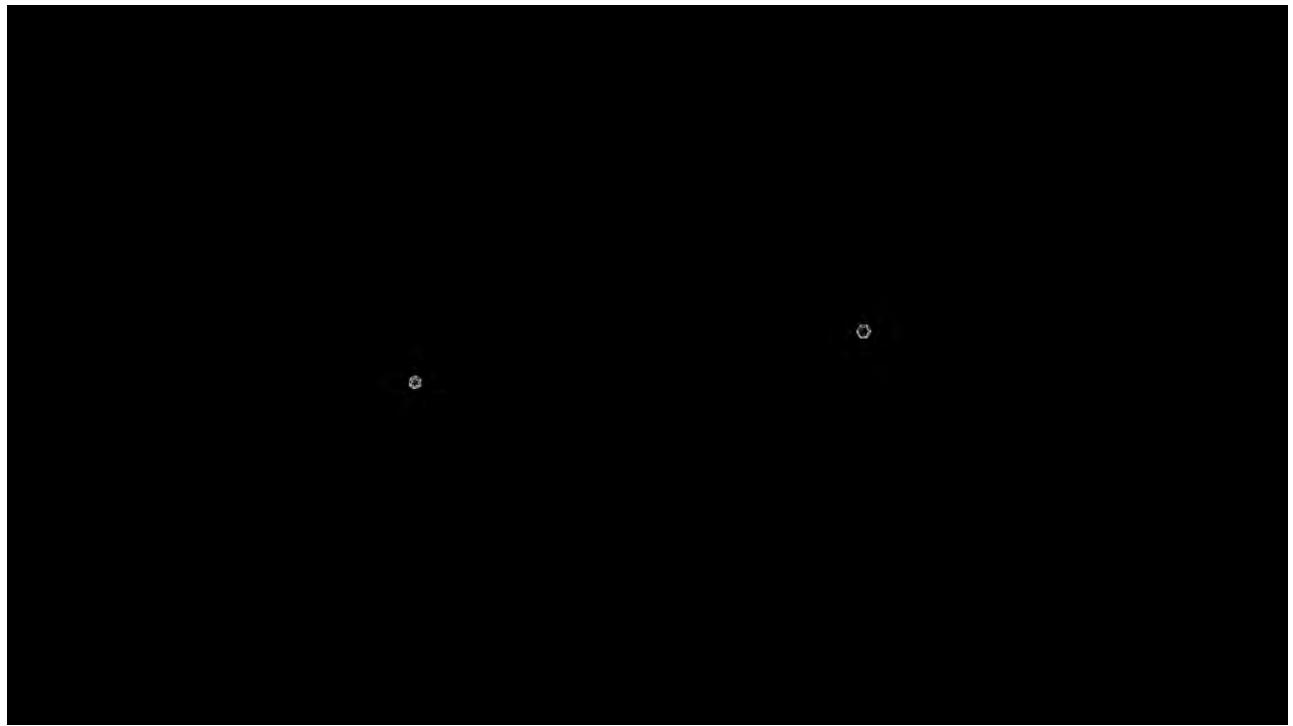
ANSWER THE QUESTION ON BLUE SCREEN IN ONE MOMENT



How long does it take to grow a typical stellar crystal in the atmosphere?

- 2 minutes
- 10 minutes
- 30 minutes
- 2-3 hours
- 24 hours

* If your answer differs greatly from the choices above tell us in the chat!



For more pictures, more movies, more science ... see *SnowCrystals.com*

The screenshot shows the homepage of SnowCrystals.com. At the top right is a large blue snowflake. To its left is a smaller image of two snowflakes. Below these are four more snowflake images arranged in a grid. The central text reads "SNOW CRYSTALS .COM". A quote by Henry David Thoreau follows: "How full of the creative genius is the air in which these are generated! I should hardly admire more if real stars fell and lodged on my coat." Below the quote is the text "Welcome to SnowCrystals.com! Your online guide to snowflakes, snow crystals, and other ice phenomena". Navigation links include "PHOTOS", "BOOKS", and "SCIENCE". A book cover titled "The SNOWFLAKE: WATER'S FROZEN ARTISTRY" by Kenneth G. Libbrecht is shown. The arXiv identifier "arXiv:1910.06389" is at the bottom left.

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The banner is for an ACS Pharmacology & Translational Science webinar. It features a background image of a neuron-like cell structure with colorful, glowing filaments. The text "ACS Pharmacology & Translational Science" is in the top left, and "ACS Chemistry for Life®" is in the top right. The main title is "How to Detect and Target Dormant CANCER CELLS Surviving Microtubule-Targeting Agents". At the bottom left is a red play button icon with the word "FREE" next to it, followed by the text "Thursday, February 13 at 2pm ET". At the bottom right is a microphone icon with the text "ACS Webinars® CLICK • WATCH • LEARN • DISCUSS".

<https://www.acs.org/content/acs/en/acs-webinars/technology-innovation/microtubule-targeting-agents.html>

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A screenshot of the ACS Exams website. On the left is the cover of the 'JOURNAL OF CHEMICAL EDUCATION' Volume 81 Number 1 January 2012. In the center is the 'ACS Exams' logo with the text 'ACS Division of Chemical Education Examinations Institute'. To the right are sections for 'Instructors' and 'Students' with lists of resources. A pencil is shown pointing at a sample exam question.

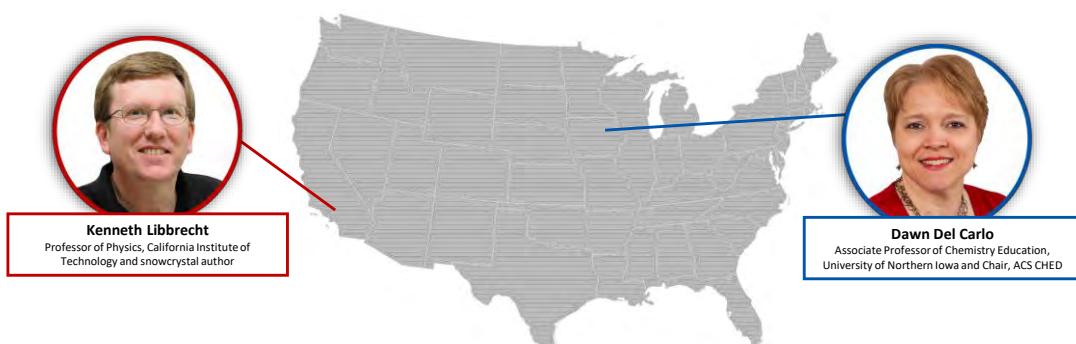
<https://pubs.acs.org/journal/iceda8>

<http://divched.org> (NEW Website coming this March!)

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The Secret Lives of Snowflakes: Peculiarities in the Molecular Dynamics of Ice Crystal Growth



Kenneth Libbrecht
Professor of Physics, California Institute of Technology and snowcrystal author

Dawn Del Carlo
Associate Professor of Chemistry Education,
University of Northern Iowa and Chair, ACS CHED

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