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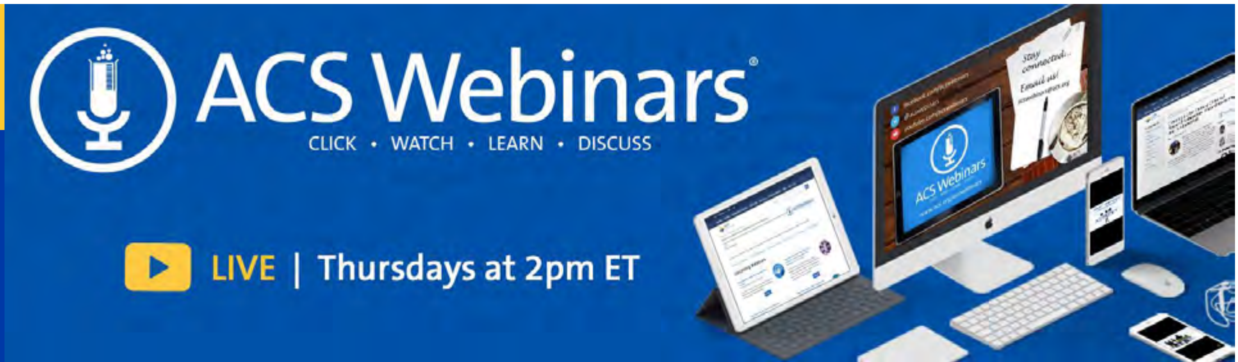

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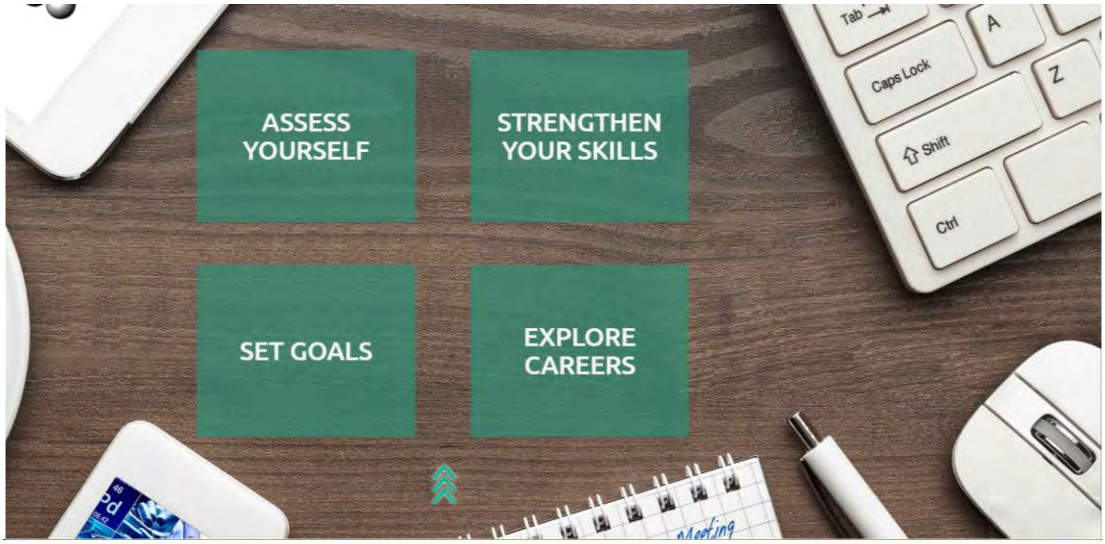

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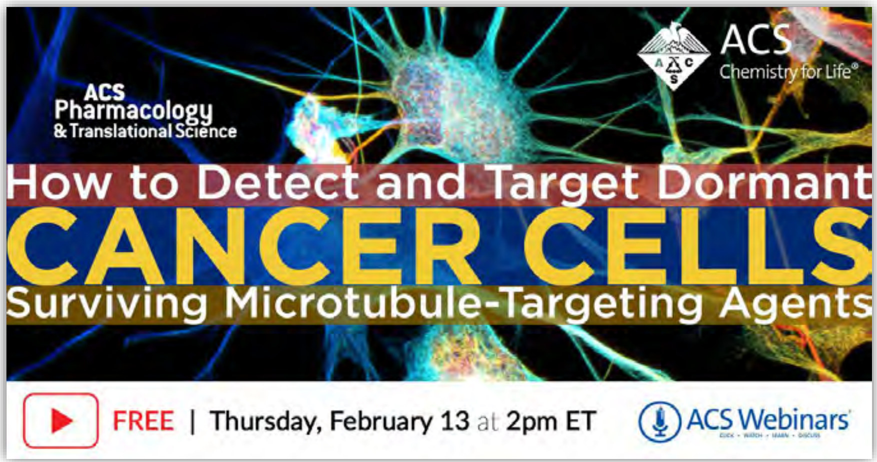

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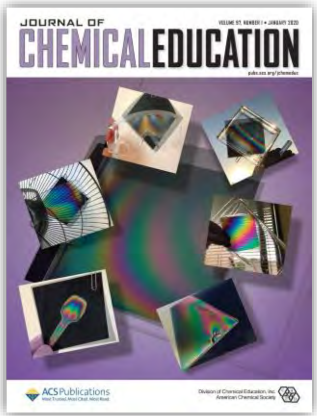

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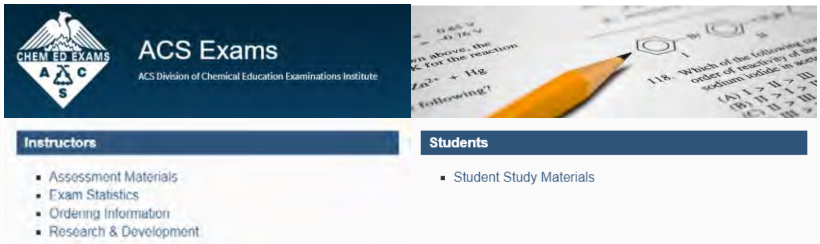

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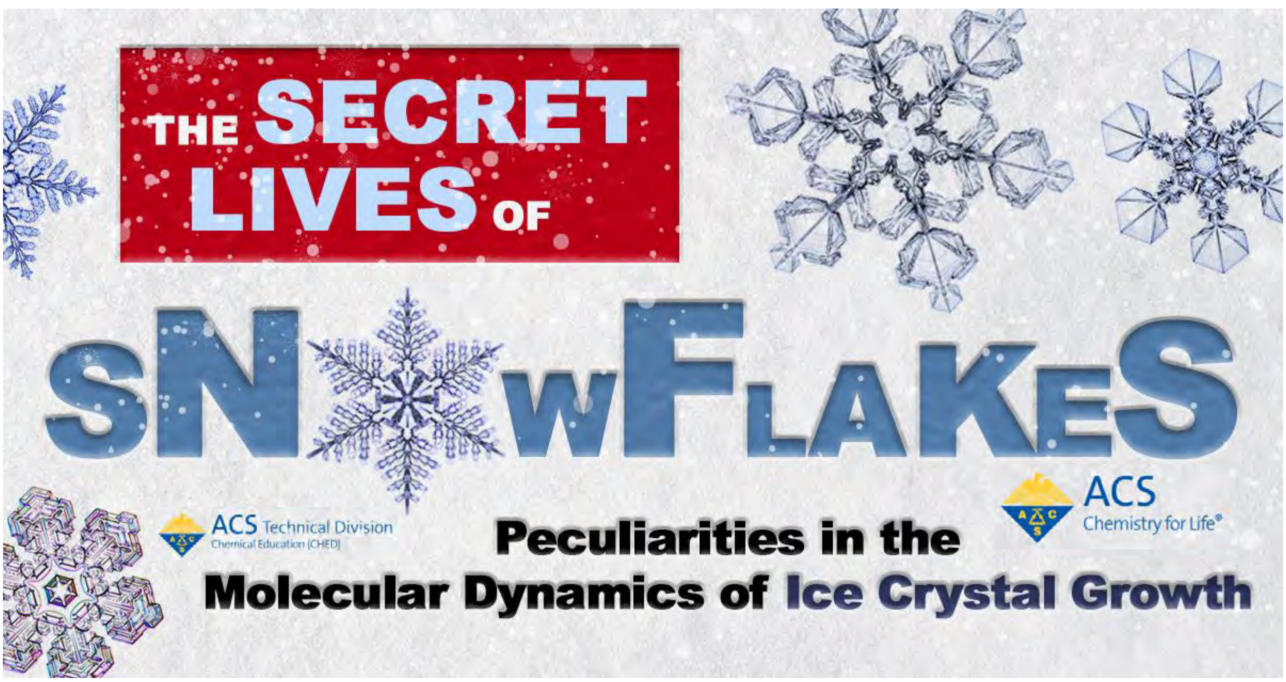

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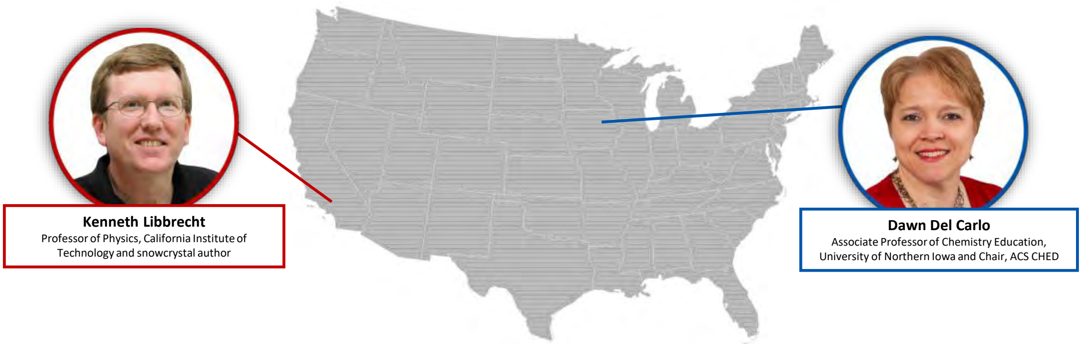
ACS Chemistry for Life®

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



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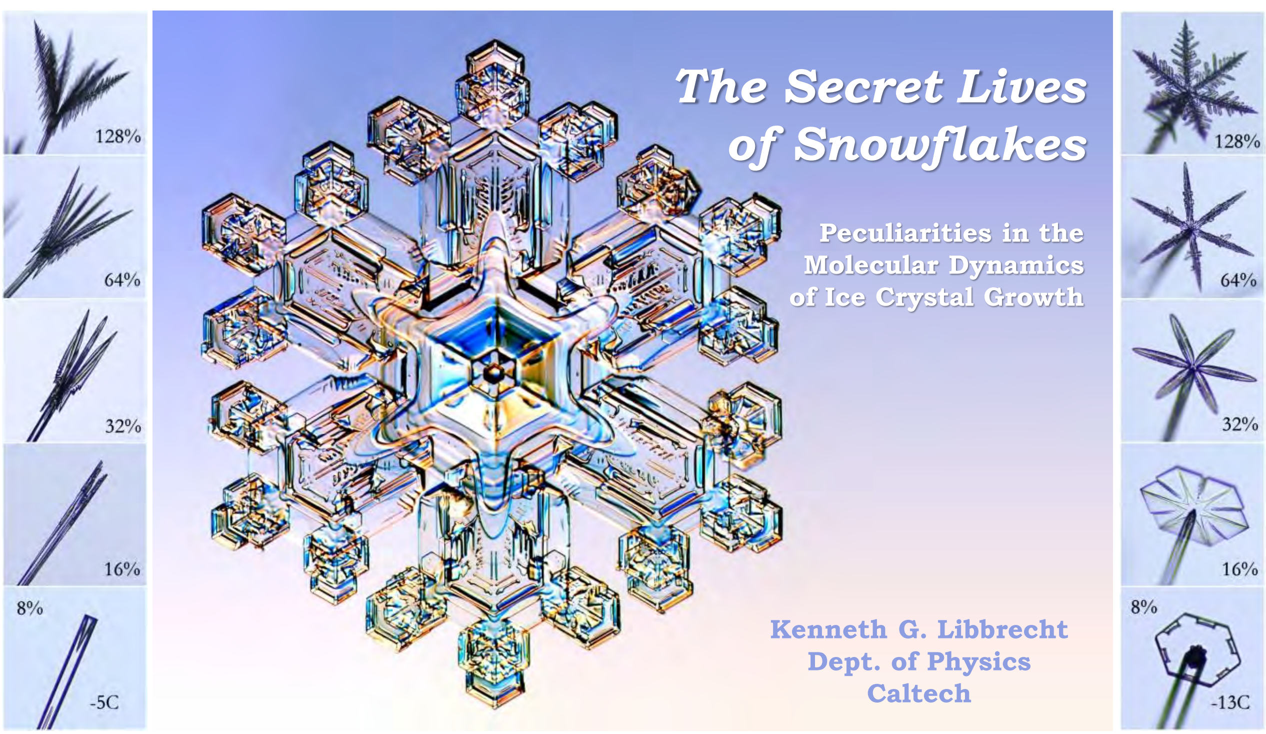
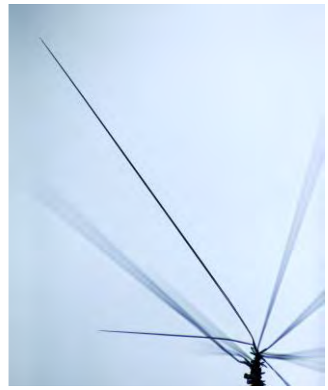


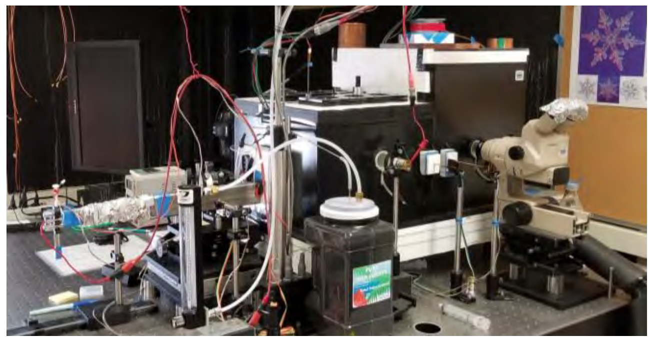
A laboratory "Snowflake on a Stick"

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, σ = 16%
then 64%





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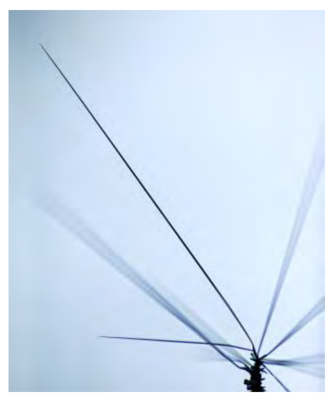
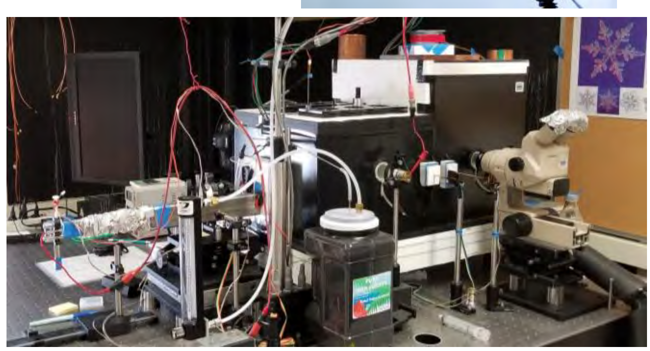
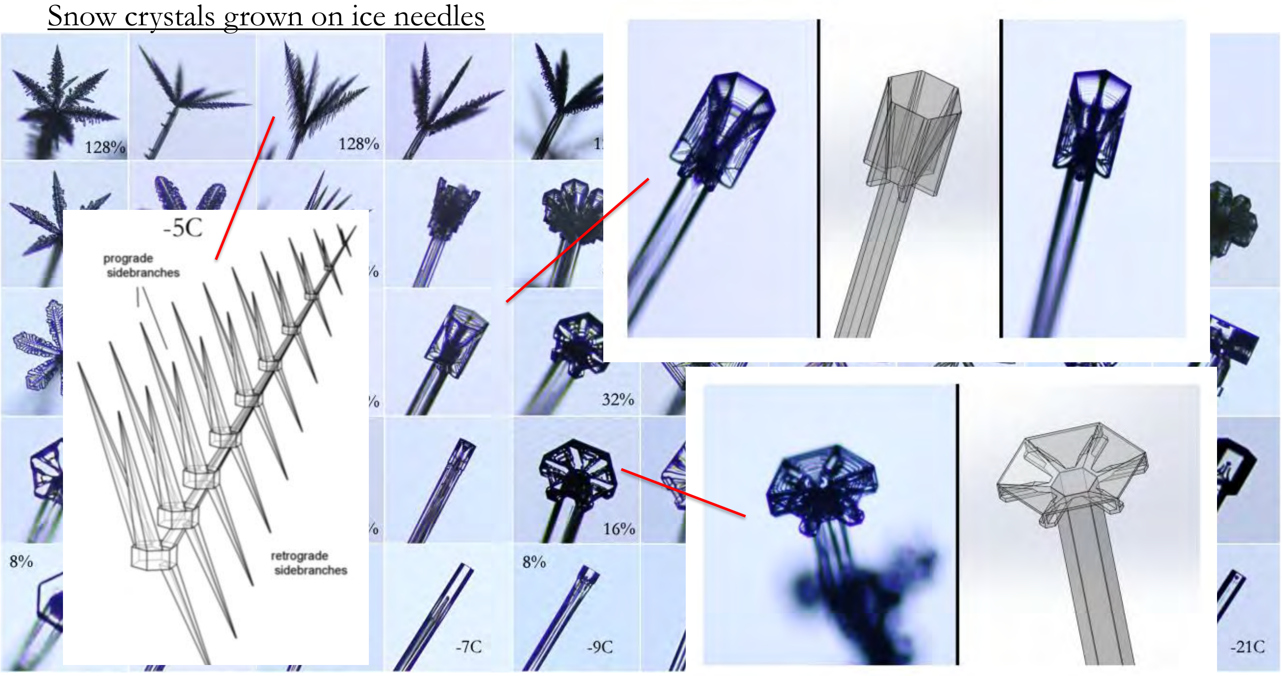




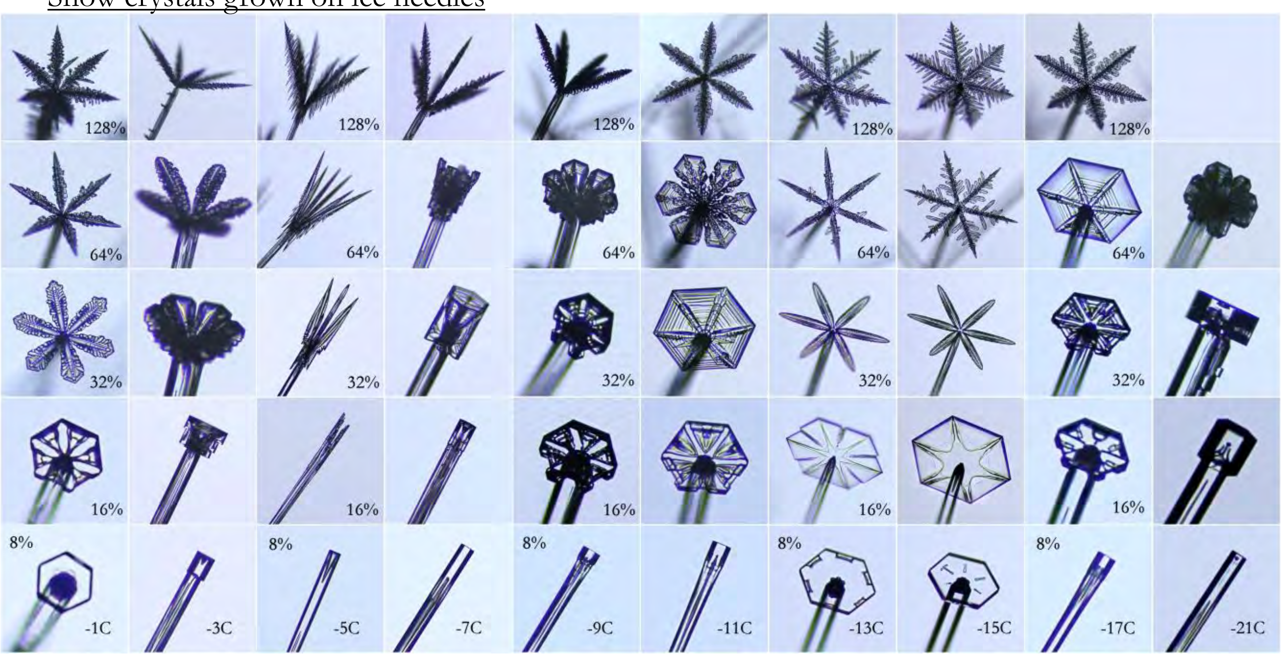
Snow crystals grown on ice needles



Unusual behavior as function of temperature

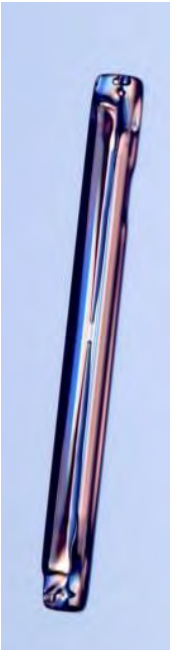
All single crystals; all grown at constant conditions

Snow crystals grown on ice needles



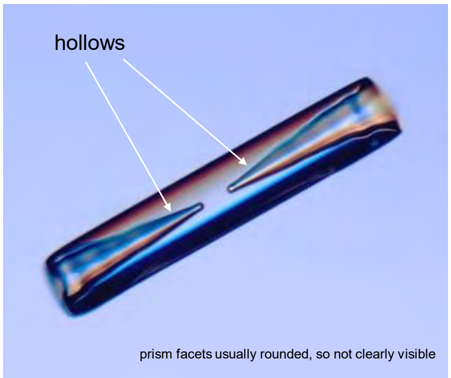
What is the underlying physics? Can make computer models?

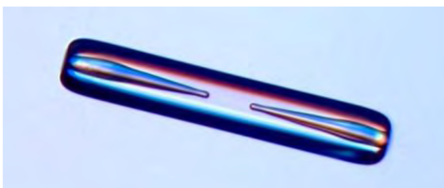
Can find these in nature also…

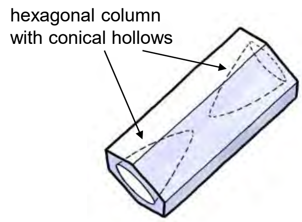


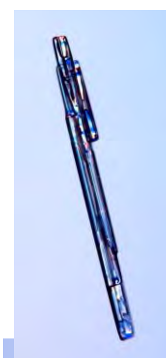
Natural Snow Crystals...

Hollow Columns, form at -5C



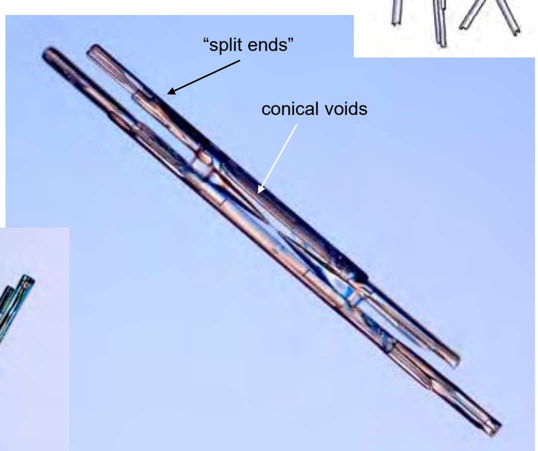




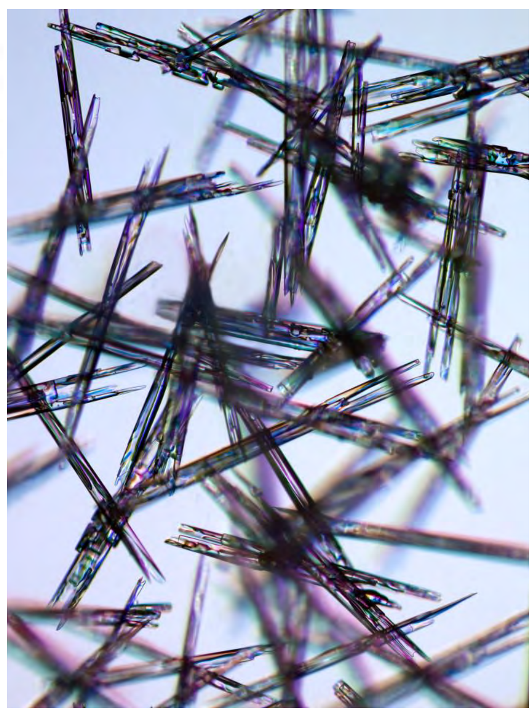


Natural Snow Crystals...

Needle Crystals, form at -5C



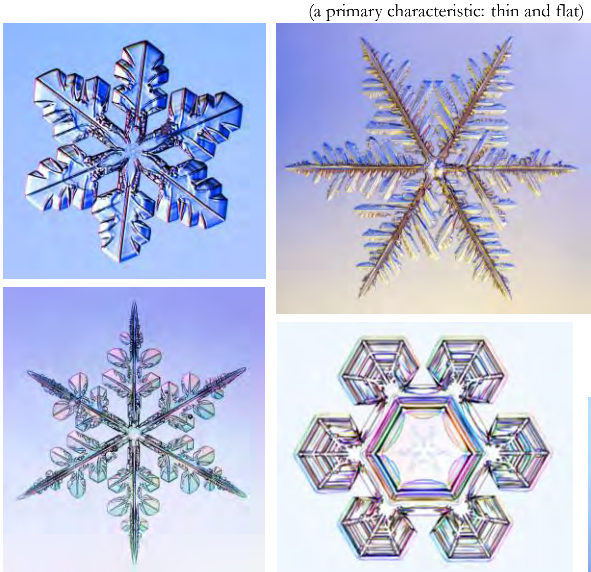
longest columnar crystals 2-3 mm
often find in clusters



Natural Snow Crystals...

Stellar Crystals, form at -15C

(a primary characteristic: thin and flat)



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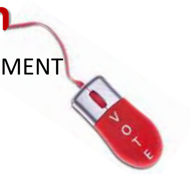
Audience Survey Question

ANSWER THE QUESTION ON BLUE SCREEN IN ONE MOMENT



How large are typical stellar snow crystals in nature?

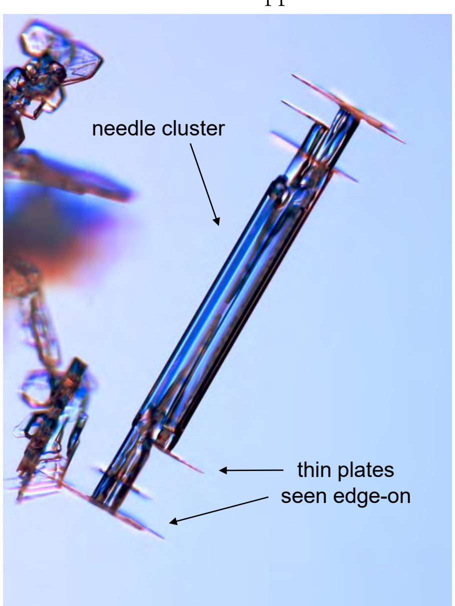
- About 0.1 millimeters from tip to tip
- About 0.3 millimeters
- About 1 millimeter
- About 3 millimeters
- About 10 millimeters

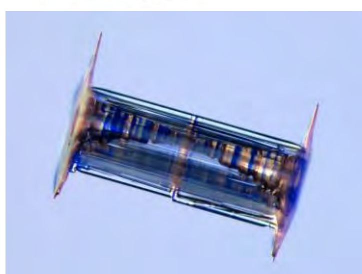
** If your answer differs greatly from the choices above tell us in the chat!*

<u>Natural Snow Crystals...</u>
Size comparisons

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

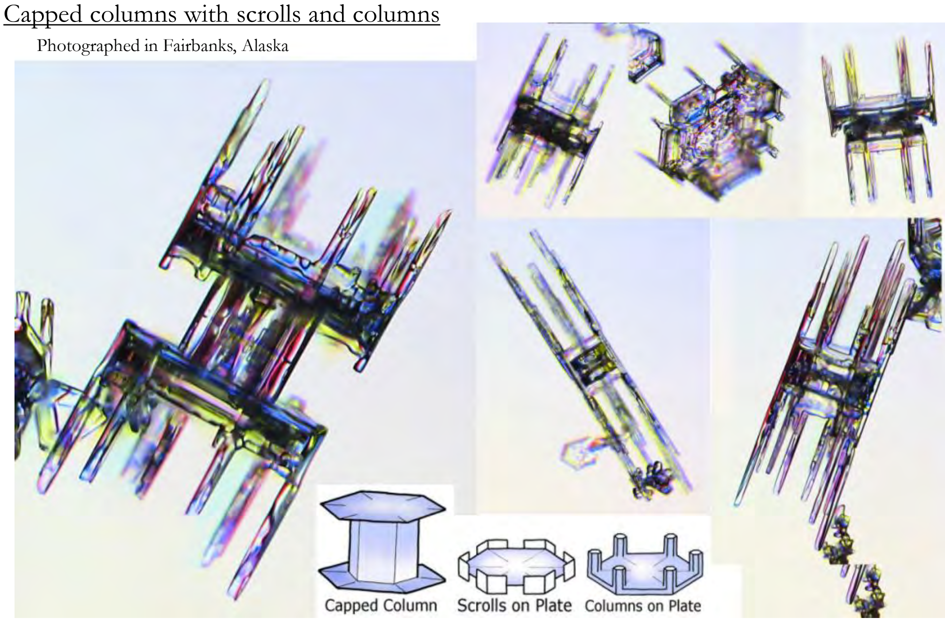
<u>Natural Snow Crystals...</u>
Capped Columns



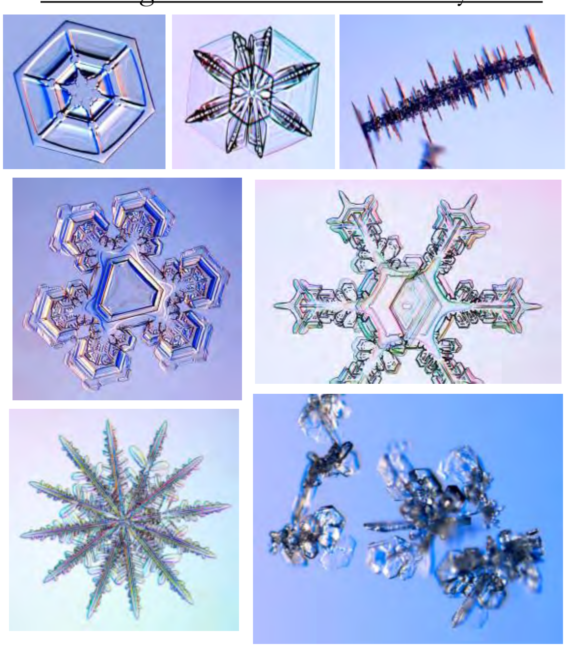


Some especially odd examples:
Capped columns with scrolls and columns

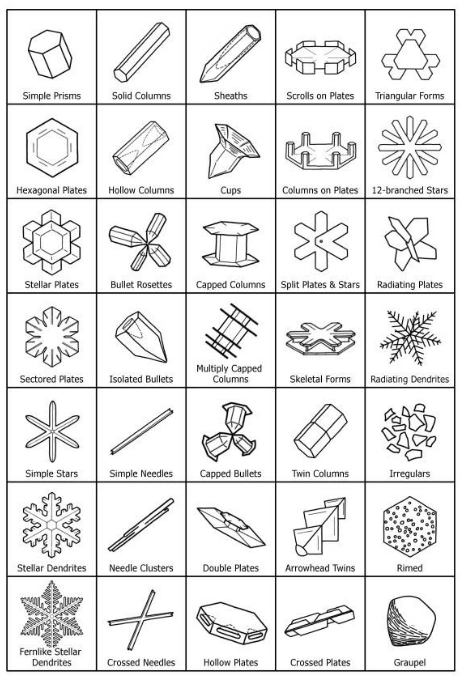
Photographed in Fairbanks, Alaska



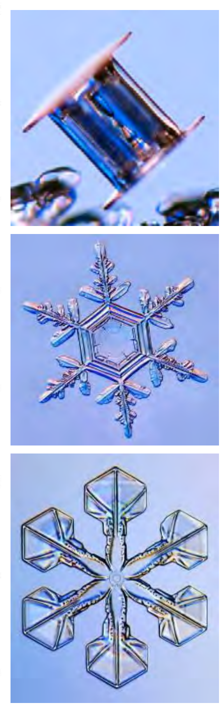
A Menagerie of Natural Snow Crystals...



What is the underlying physics?



from *Ken Libbrecht's Field Guide to Snowflakes*

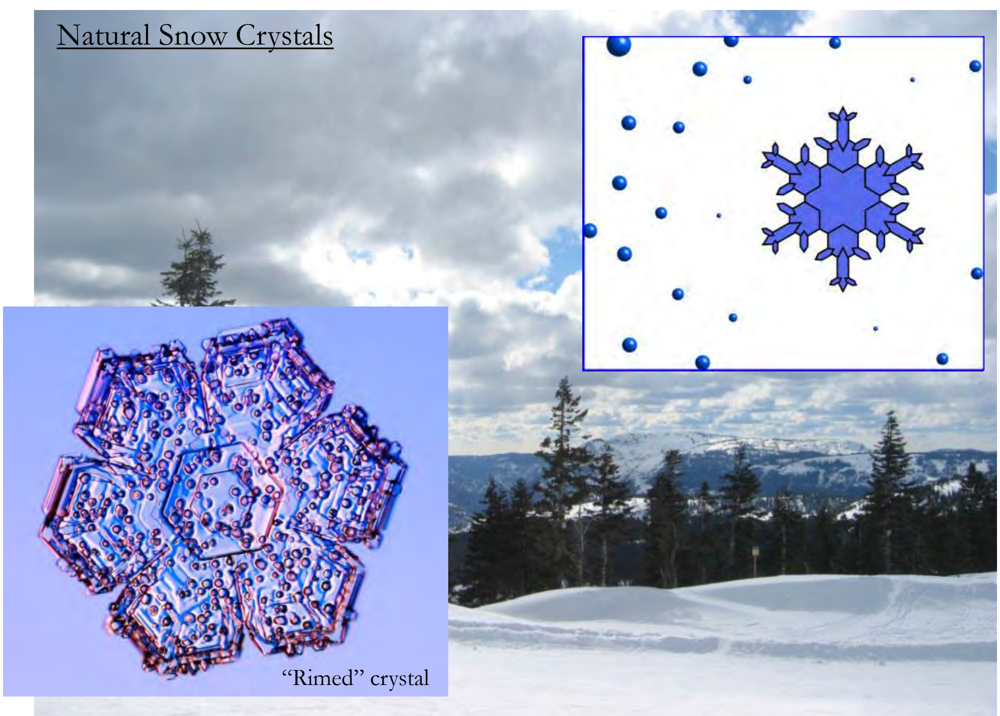


The wrong way to make a snowflake

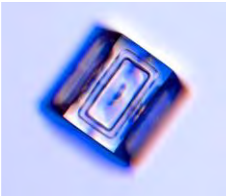
Christopher Buchholz

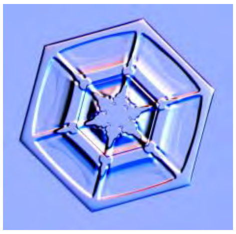
Nature makes things using self-assembly...

Natural Snow Crystals



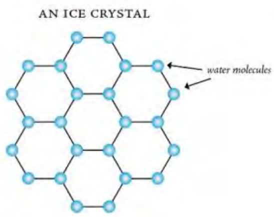
"Rimed" crystal

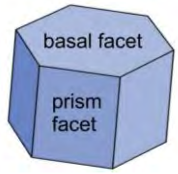


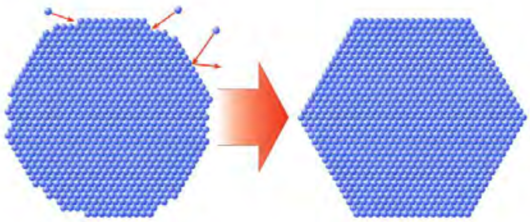


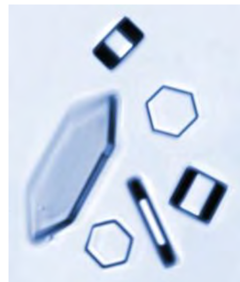
Snowflake Physics I - Faceting

Structure of the Ice Crystal → Facets









Tiny, laboratory grown snow crystals ~0.1 mm

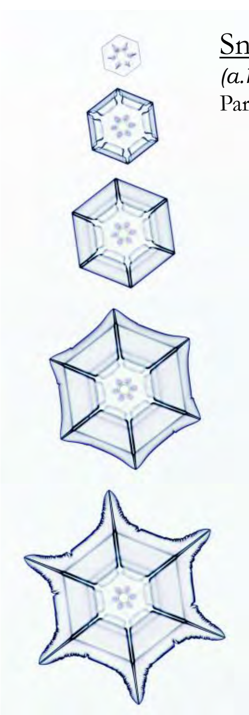
Attachment Kinetics
(highly anisotropic)

(Surface energy not very important; nearly isotropic)

Molecules cannot readily attach to smooth surfaces
→ facets form as crystal grows

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

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

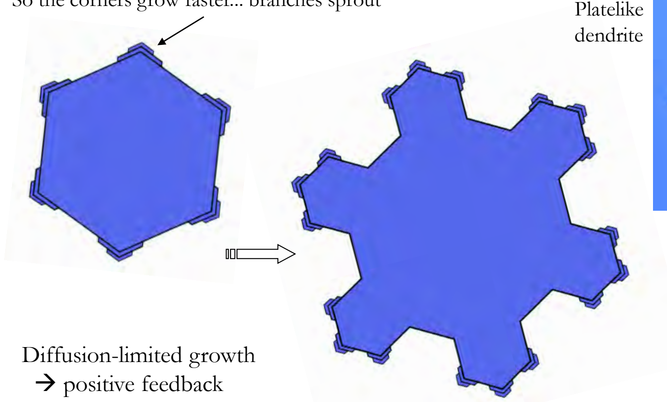


Snowflake Physics II – The Branching Instability

(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

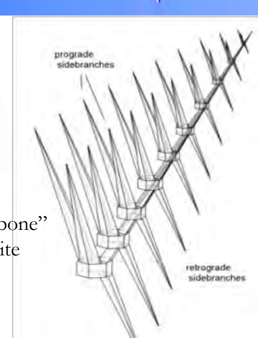


Platelike dendrite

Diffusion-limited growth
→ positive feedback
→ growth instability
→ branching, sidebranching …

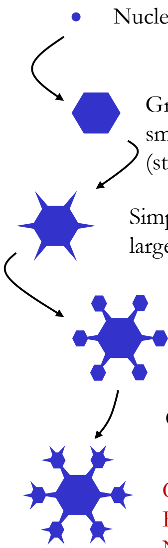
Much scientific literature on diffusion-limited growth

"Fishbone" dendrite



Snowflake Physics III - Complexity and Symmetry

(an explanation of the "No-Two-Alike" conjecture)



- Nucleation of ice particle

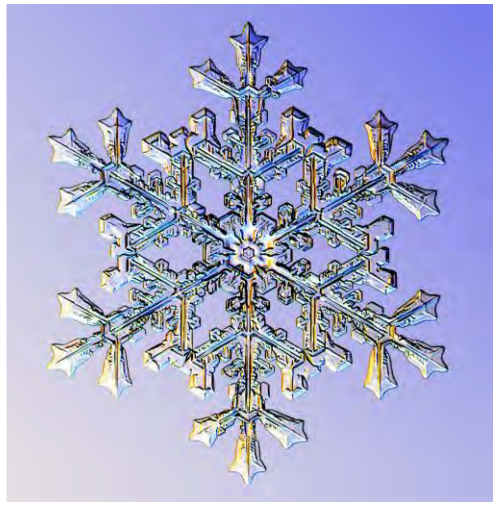
Grows to hexagonal prism, since smooth facets grow most slowly (stellar snow crystal)

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

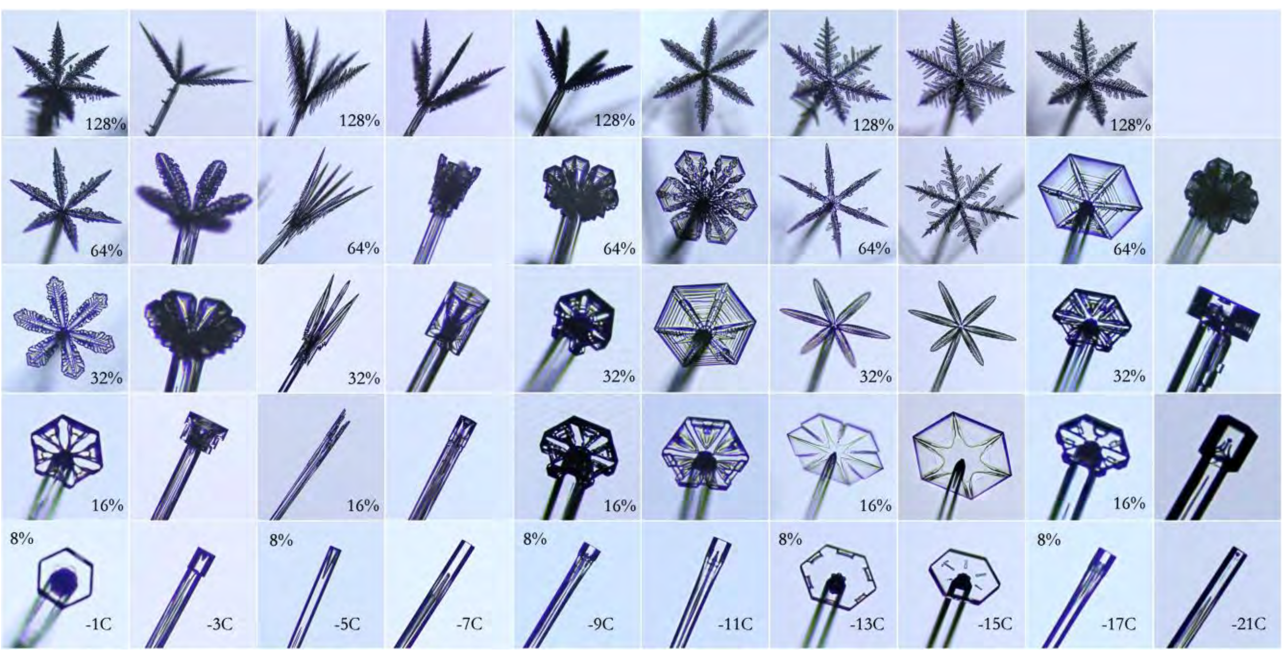
Crystal moves to different temperature ... plates grow on arms

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

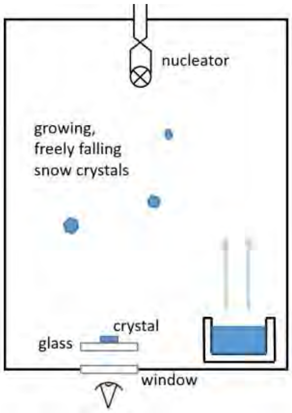
Complex history → Complex crystal shape, faceted & branched
Each arm experiences same history → Symmetry
No two paths are the same → No two alike
All because growth sensitive to temperature, humidity



T~ -1 C → Platelike   T~ -5 C → Columnar   T~ -15 C → Platelike

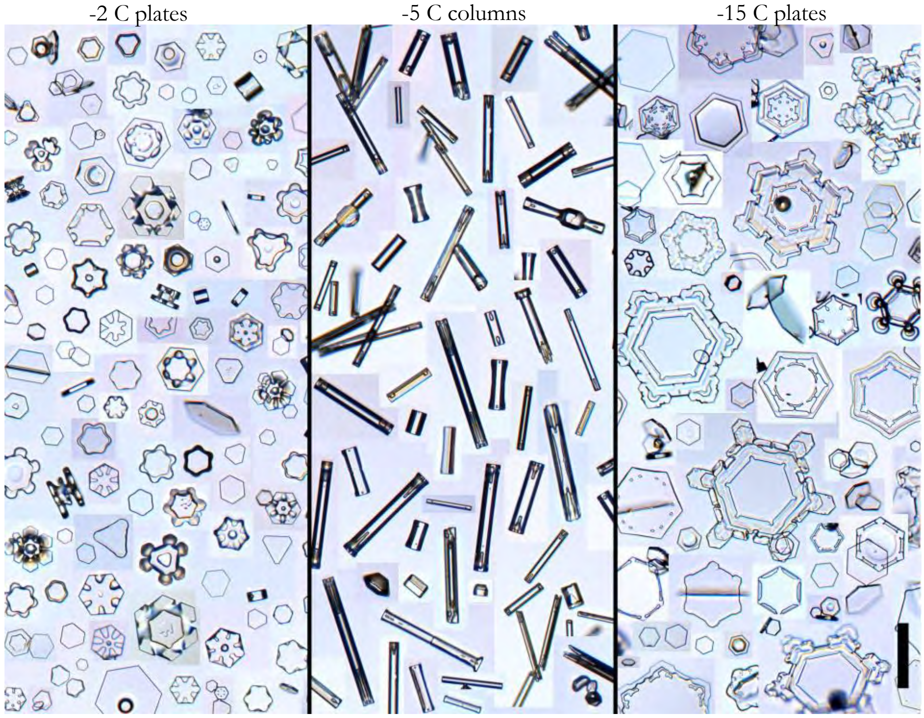


How explain morphology versus temperature and supersaturation?



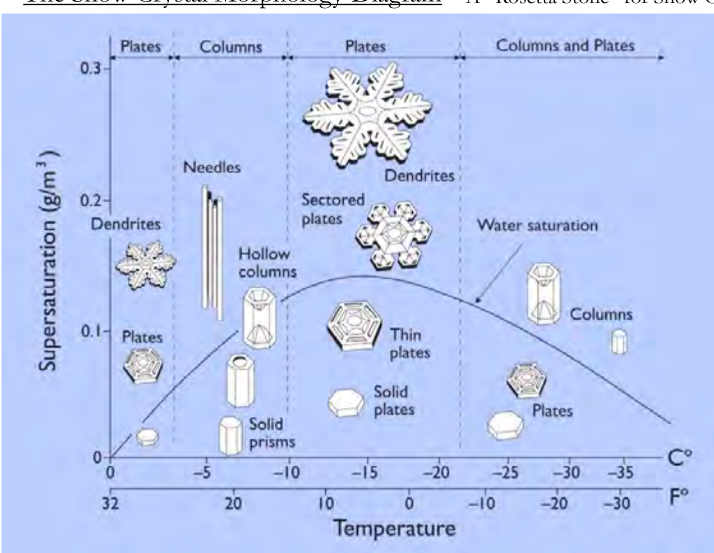
Laboratory
snow crystals
grown in free fall

-2 C plates | -5 C columns | -15 C plates



The Snow Crystal Morphology Diagram

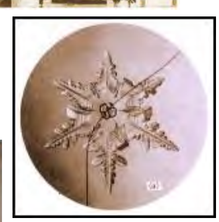
A "Rosetta Stone" for Snow Crystals

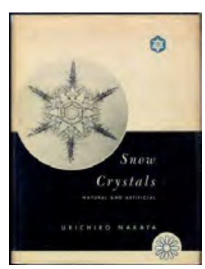


An unsolved puzzle for 65 years… a purely empirical result
Solved at last?
KGL, arXiv:1910.09067
arXiv:1910.06389

Attachment kinetics is key → Examine facet growth

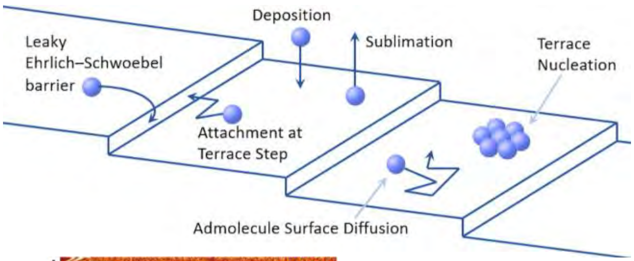
Ukichiro Nakaya
~ 1930s
Hokkaido University

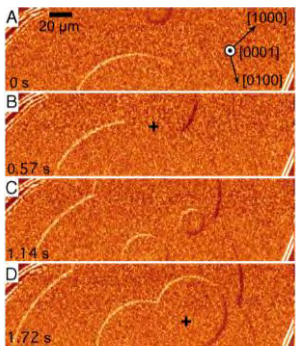




Snow Crystals, Natural and Artificial, 1954

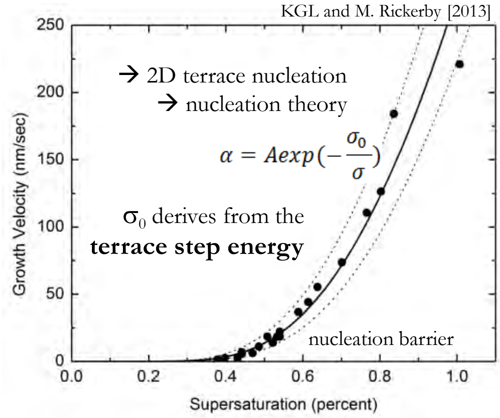
Precision Measurements of Facet growth & Step energies





Imaging Ice Terraces, Sazaki et al, 2010

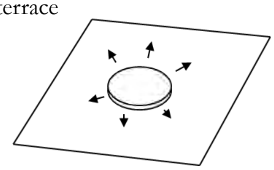
KGL and M. Rickerby [2013]



Crystal Energetics

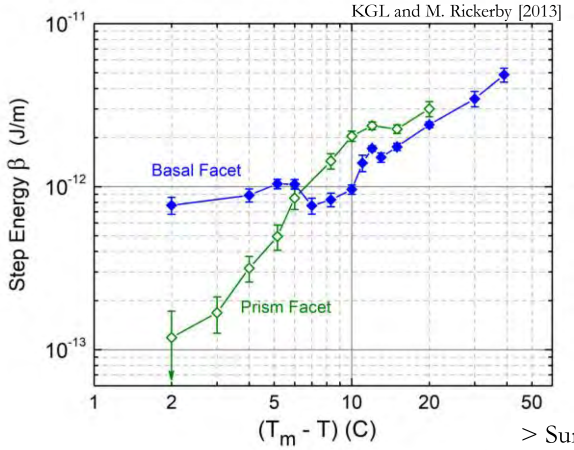
3D – latent heat (solid/vapor) … energy to vaporize crystal
2D – surface energy (tension) … energy to break bonds and create surface
1D – terrace step energy … energy to split island terrace
(on faceted surfaces)

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

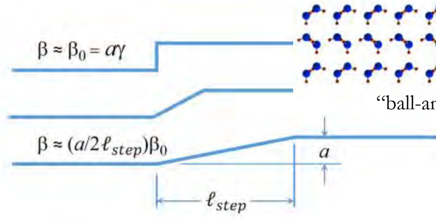


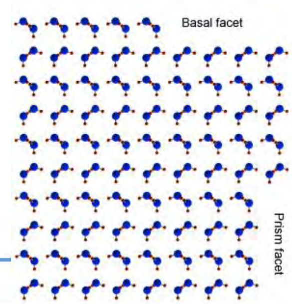
Facet growth & Step energies

KGL and M. Rickerby [2013]



> Single parameter
determines growth rates!
(nucleation barrier)





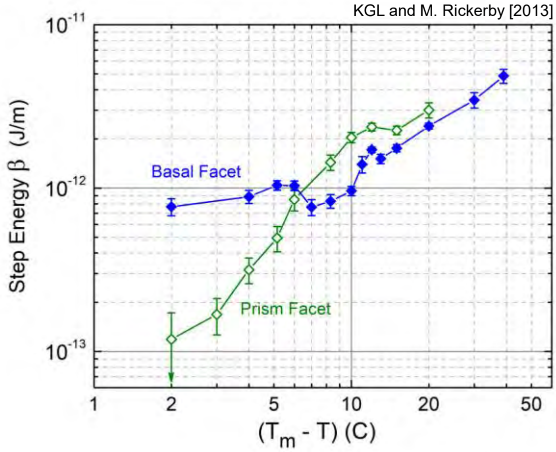
"ball-and-stick" model

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

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

> 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 …

J. P. D. Abbatt, 2003
Chemical Reviews, 2003, Vol. 103, No. 12 4785

Surface Premelting

← Quasiliquid layer (QLL)

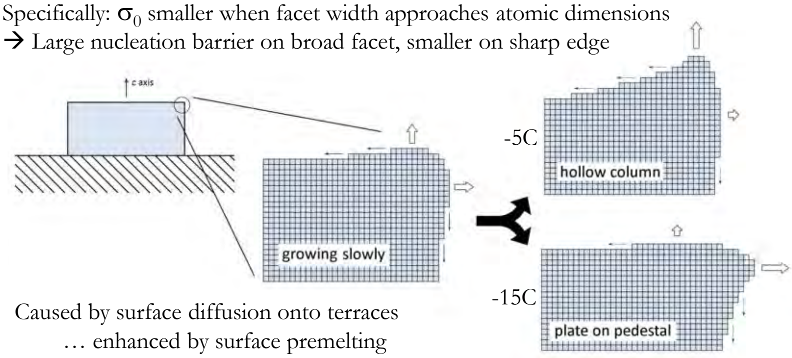
← terrace step located at ice/QLL interface

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

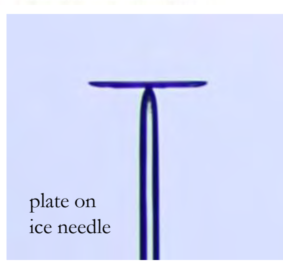
→ an *edge-sharpening SDAK instability*

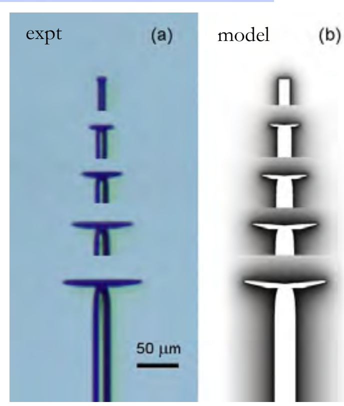
→ promotes the formation of thin plates & hollow columns

An enhanced diffusion-limited growth model

→ changes *anisotropy* of attachment kinetics

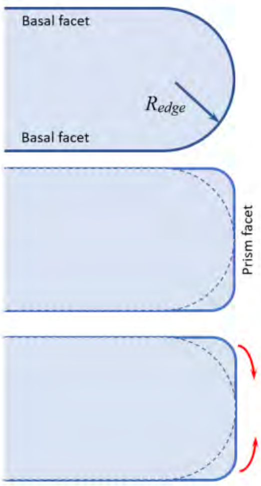
SDAK instability helps explain abrupt transitions in the morphology diagram



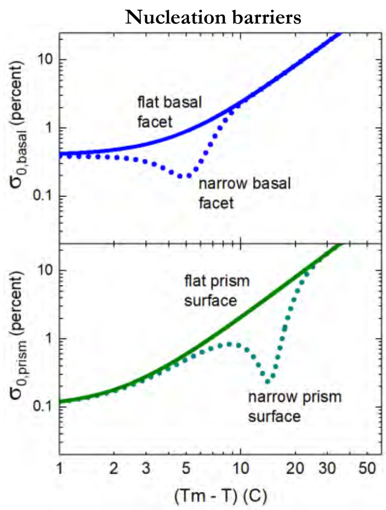


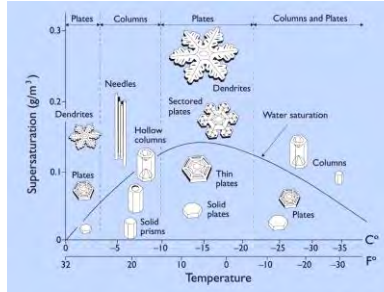
KGL arXiv:1209.4932, arXiv:1910.09067

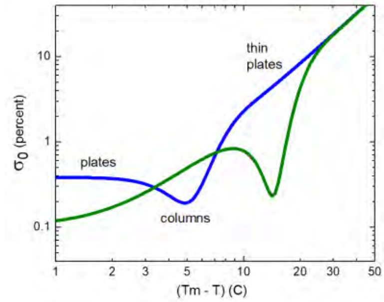
Structure Dependent Attachment Kinetics (SDAK)



Surface diffusion
from corners to facets
enhanced by surface premelting







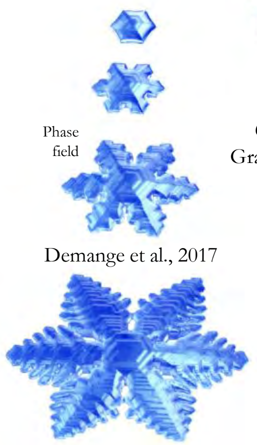
➔ A Comprehensive, *Quantitative* Model

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

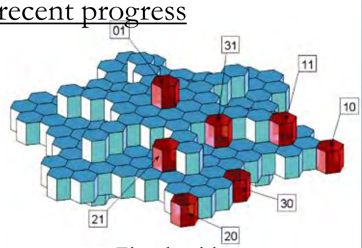
3D Numerical Modeling – lots of recent progress

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

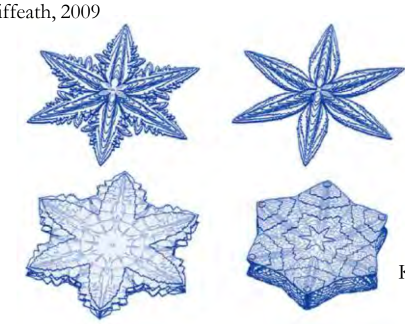
Barrett, Garcke, & Nürnberg, 2012



Demange et al., 2017



Fixed grid Cellular Automata
Gravner & Griffeath, 2009

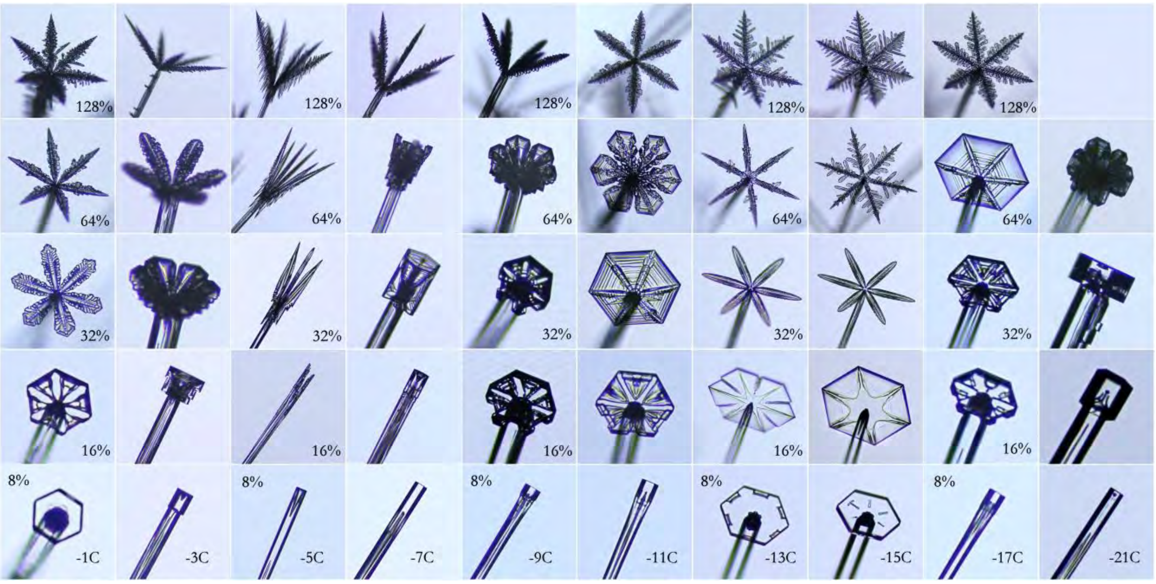


3D CA Model by David Griffeath & Janko Gravner
Rendered by Antione Clappier

Kelly &Boyer, 2014

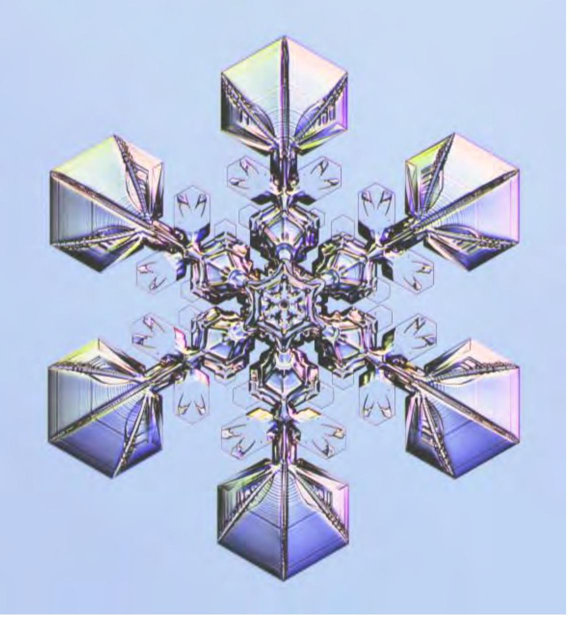
So far, morphology demonstrations only … quantitative models possible

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* …???

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



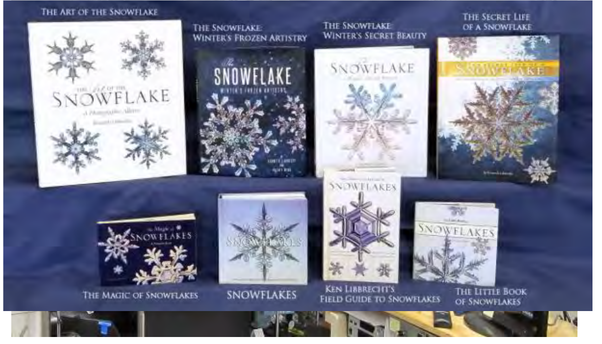
Why Ice?

overarching goal is to understand crystal growth

> 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

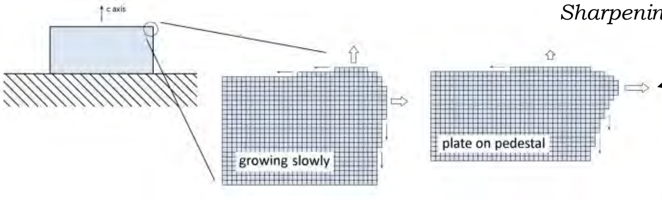
But … no (direct) applications … *zero tax dollars*

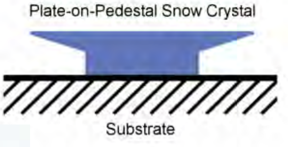
book royalties pay the bills…

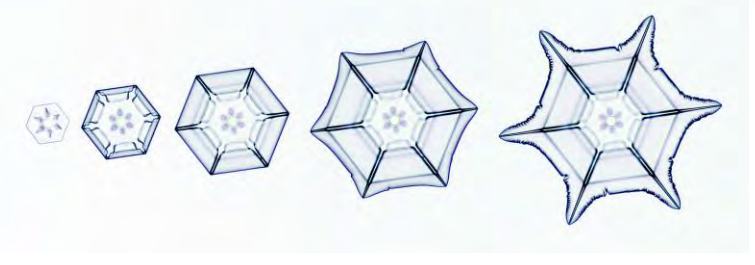


Snowflake Engineering – Plate-on-Pedestal Snow Crystals

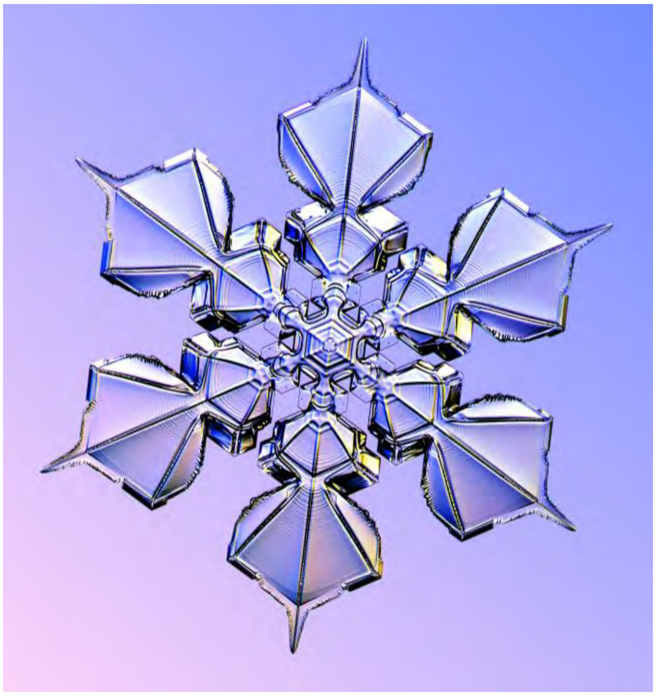
SDAK Edge Sharpening

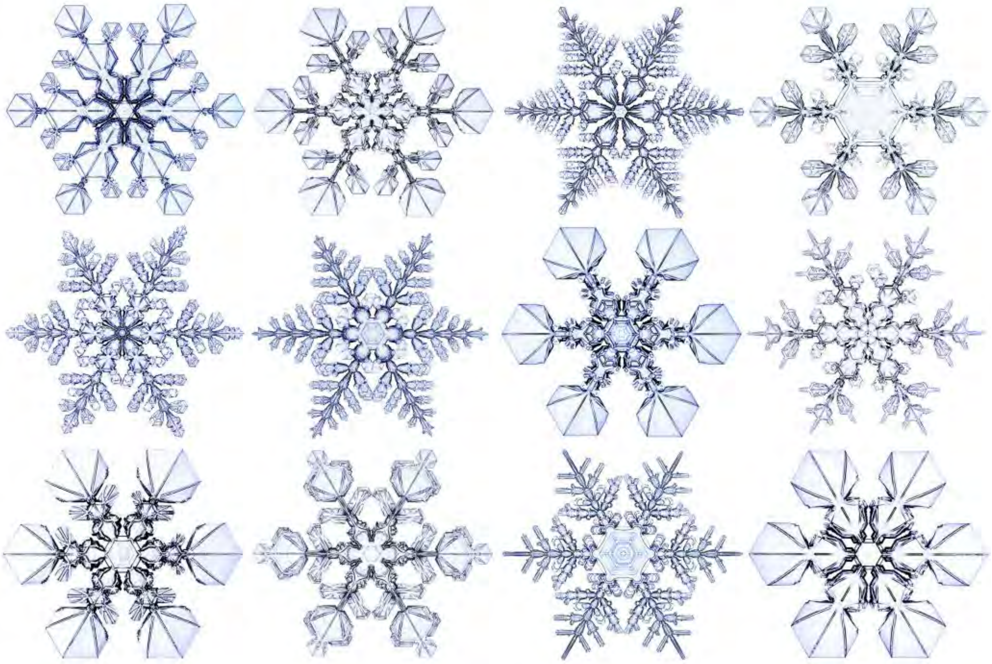


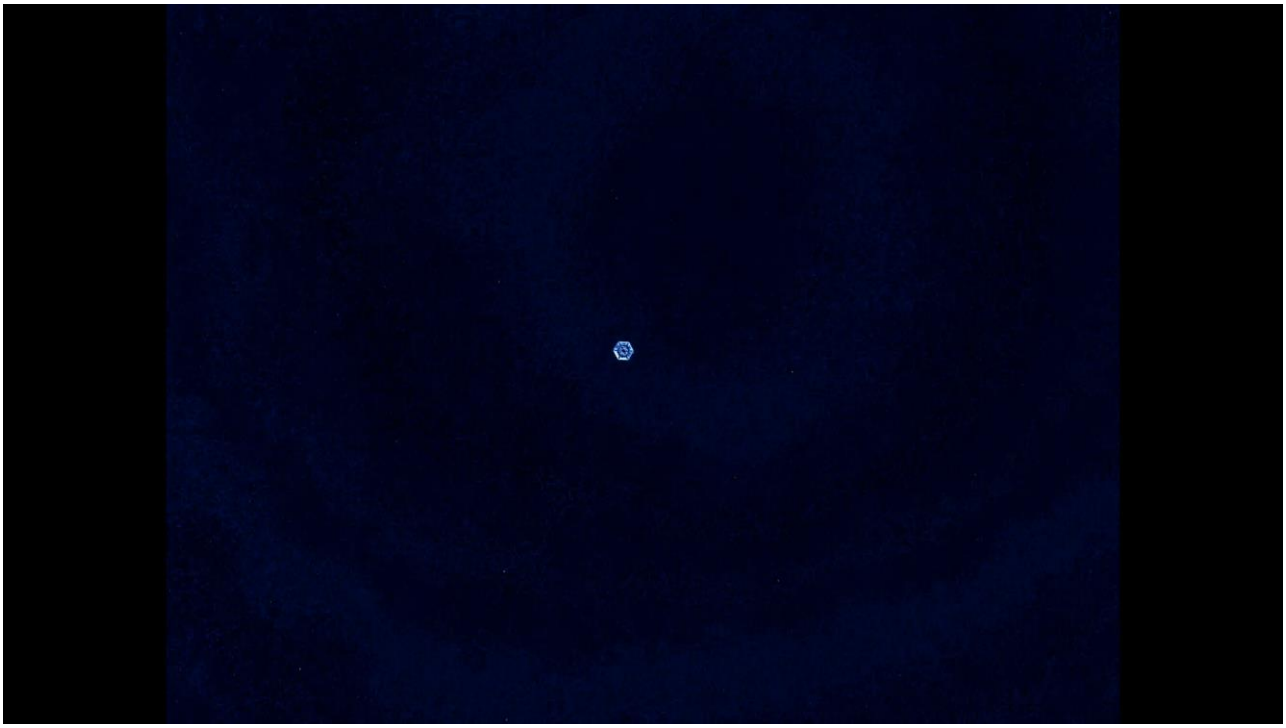




"Designer" Snowflakes

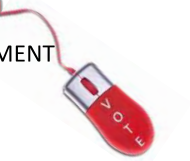


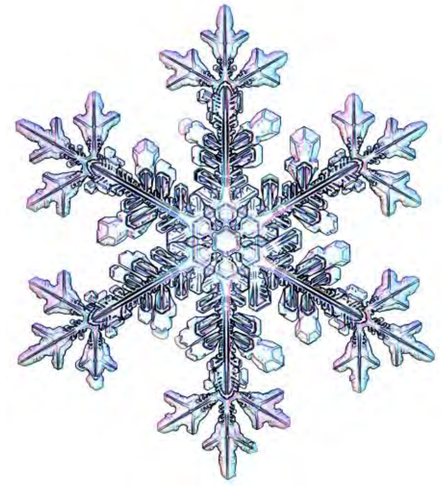




Audience Survey Question

ANSWER THE QUESTION ON BLUE SCREEN IN ONE MOMENT

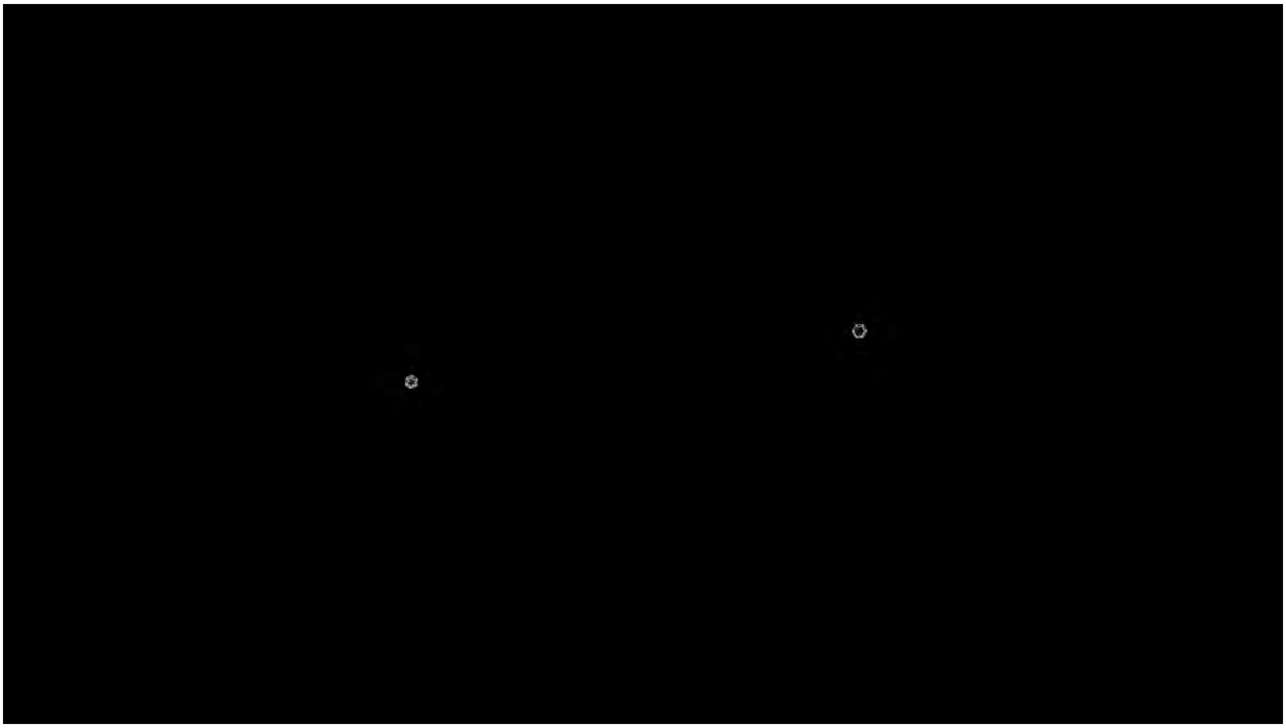


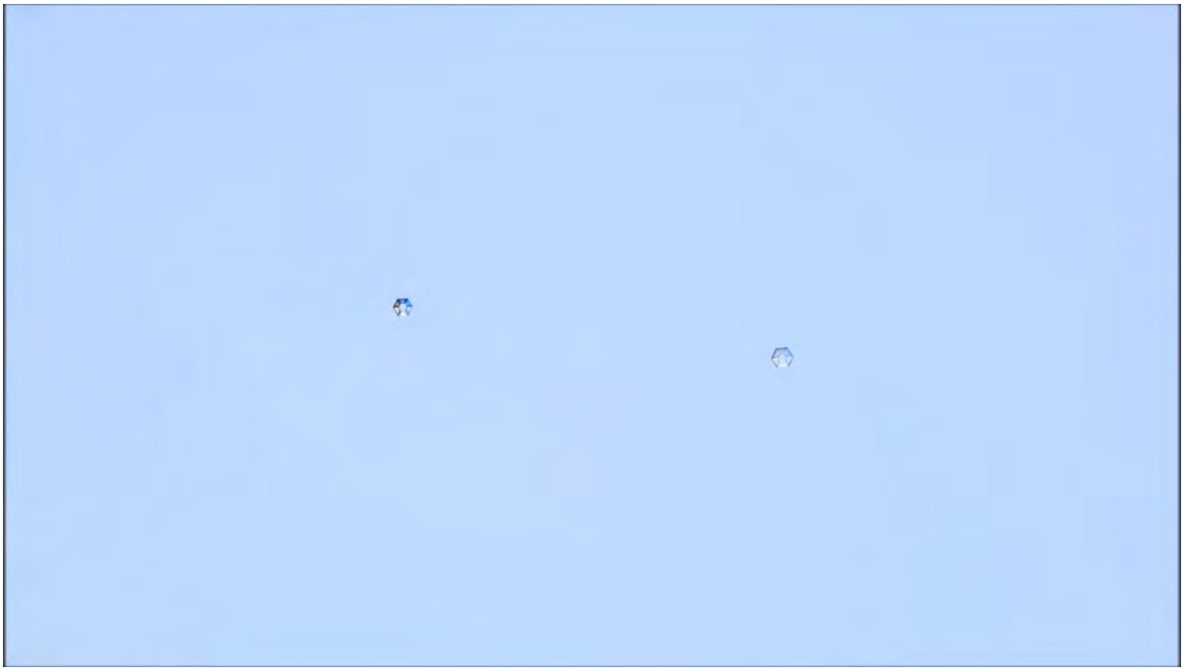


How long does it take to grow a typical stellar crystal in the atmosphere?

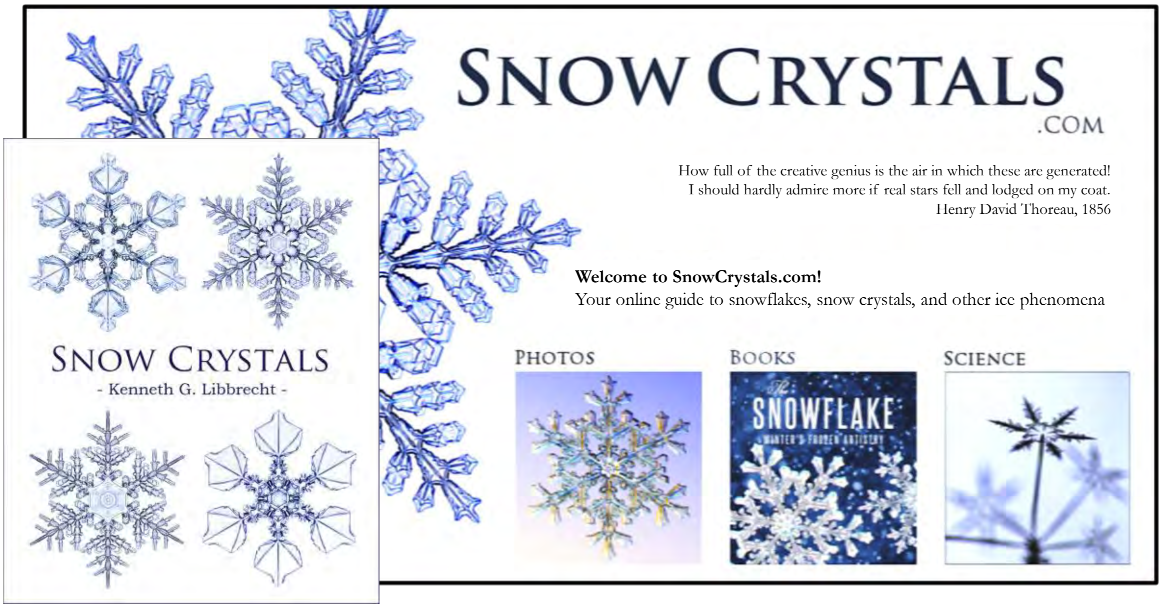
- 2 minutes
- 10 minutes
- 30 minutes
- 2-3 hours
- 24 hours

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





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



arXiv:1910.06389

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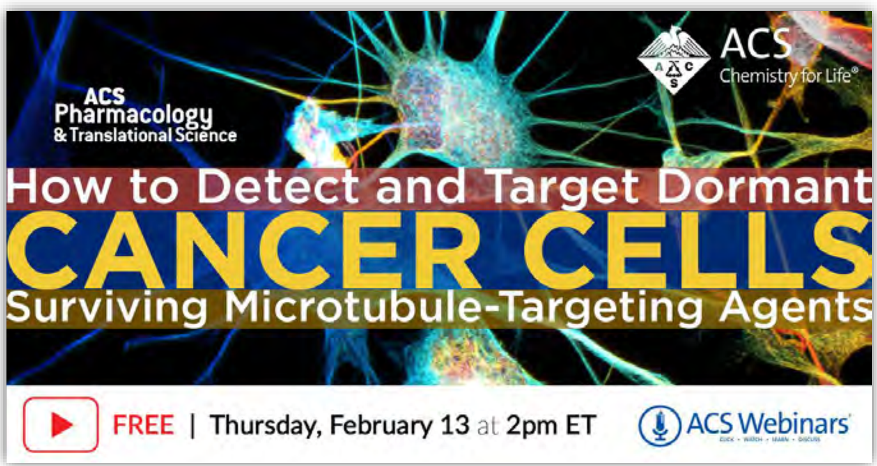

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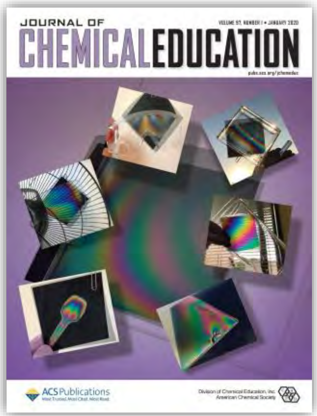

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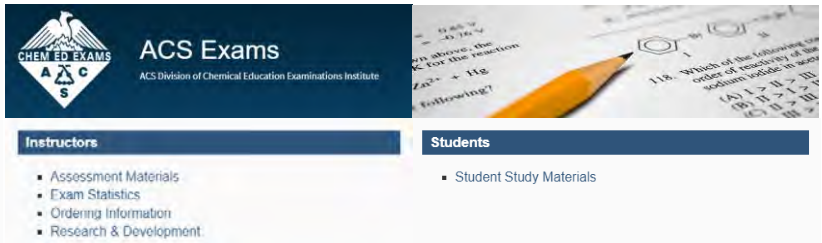

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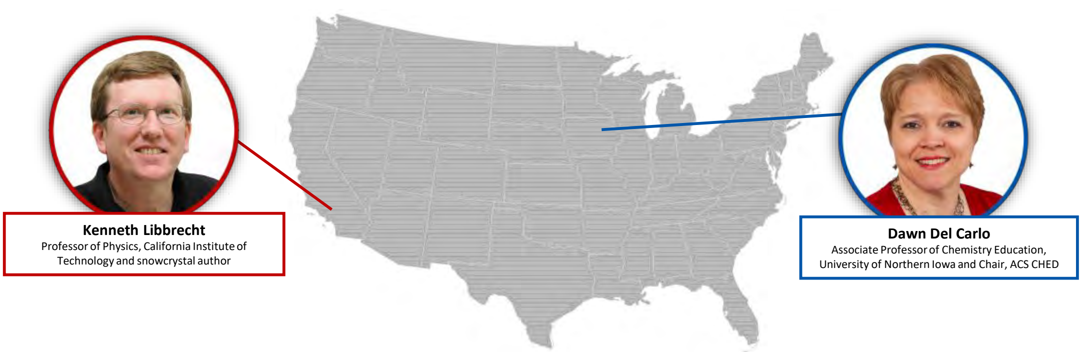

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