On modelling the formation of negative ice crystals produced by freezing of internal melt figures

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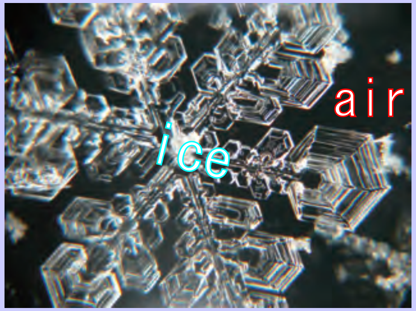
the usual ice crystals:



negative ice crystals:

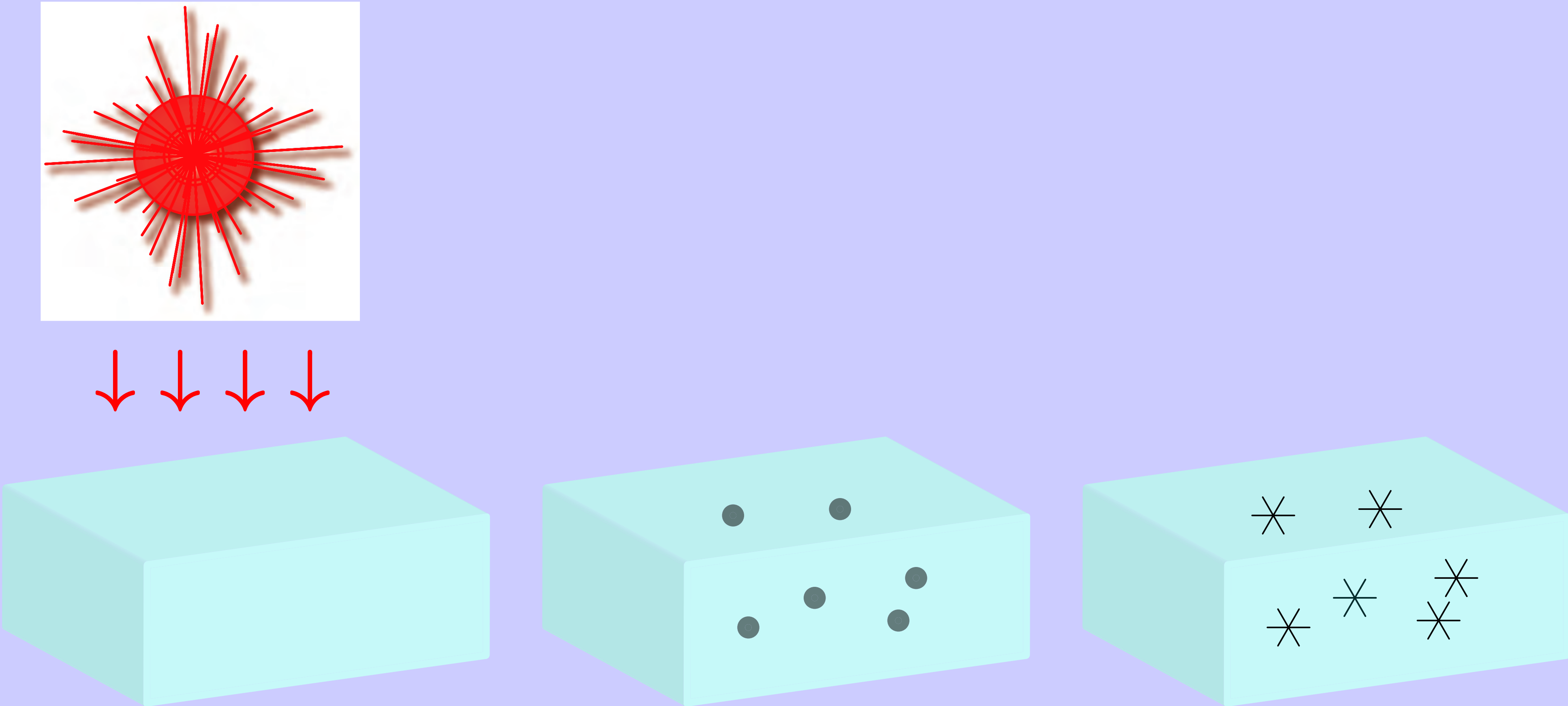
wv = water vapor

Where?

How?

Model?

Internal melting

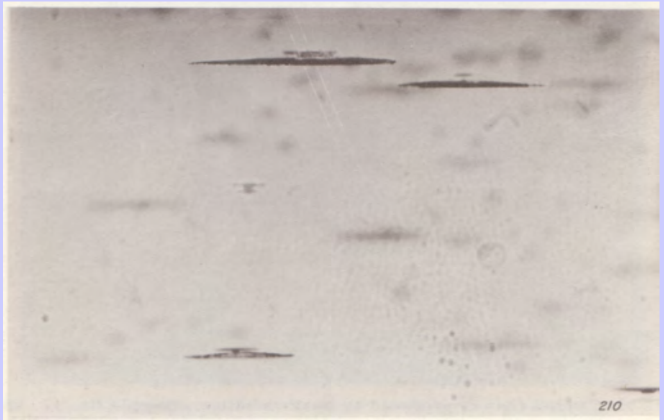


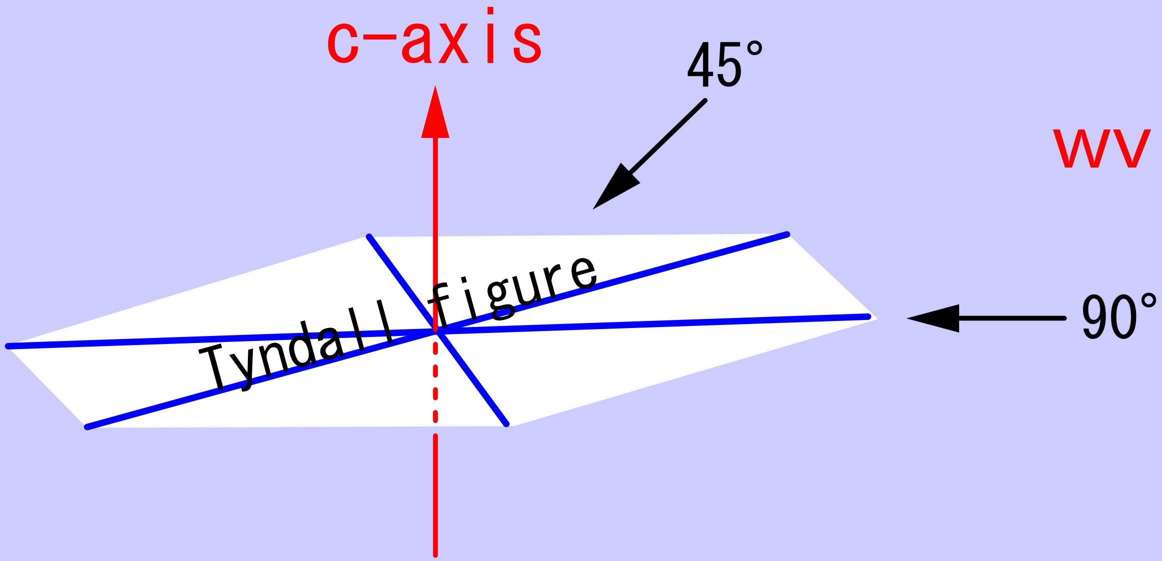
a block of ice ⇒ internal melting (without melting the exterior portions) ⇒ formation of six petals

Tyndall figures

45 °

90 °



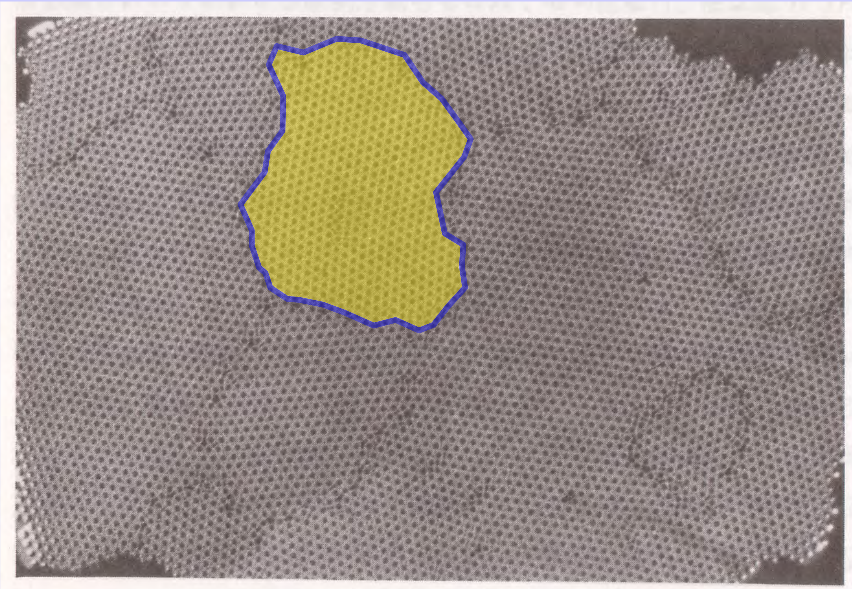


wv = water vapor saturated at that temperature

☆ Tyndall (1858) found this phenomenon at a glacier.

Properties of ice

Polycrystalline Ice



blue: grain boundary

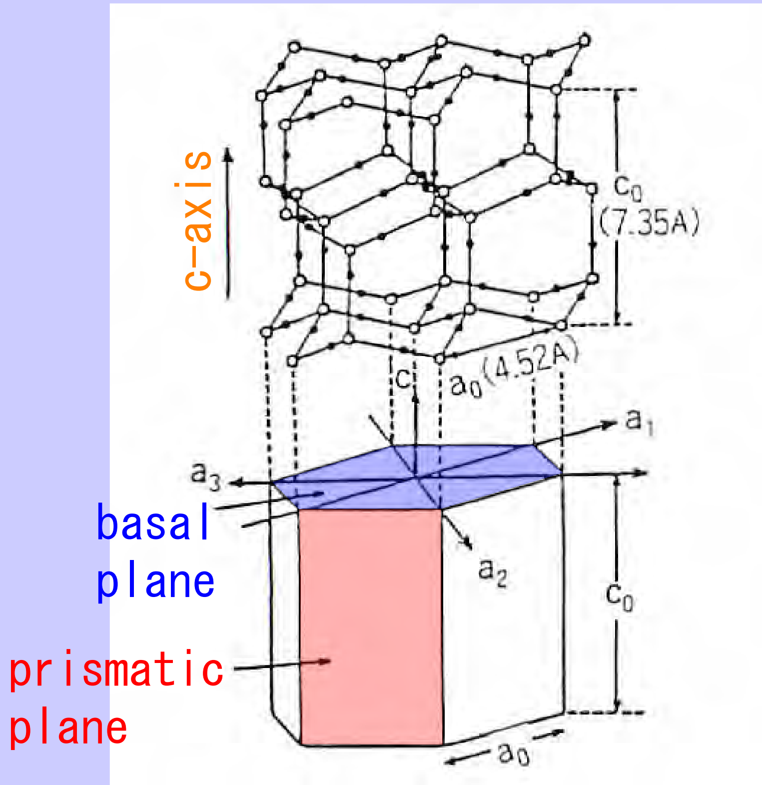
yellow: grain

= single ice crystal

<u>Lattice structure of ice</u> ⇒

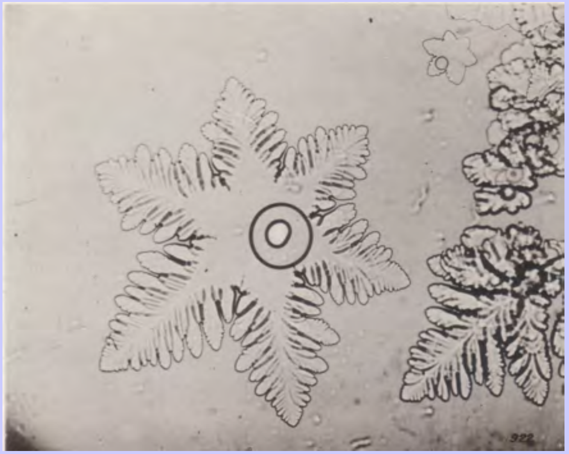
c-axis: main axis

basal plane = a regular hexagon



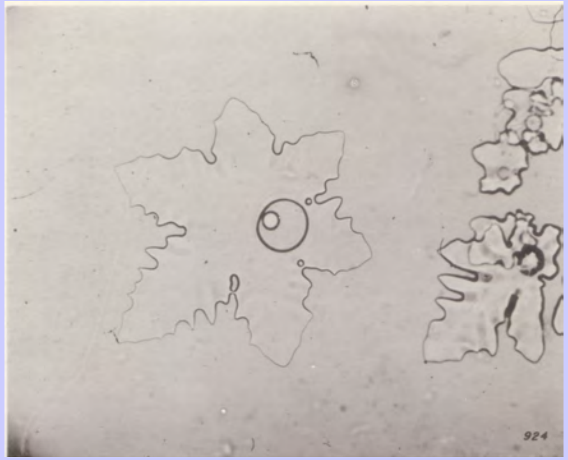
When the Tyndall figure is refrozen

all pics

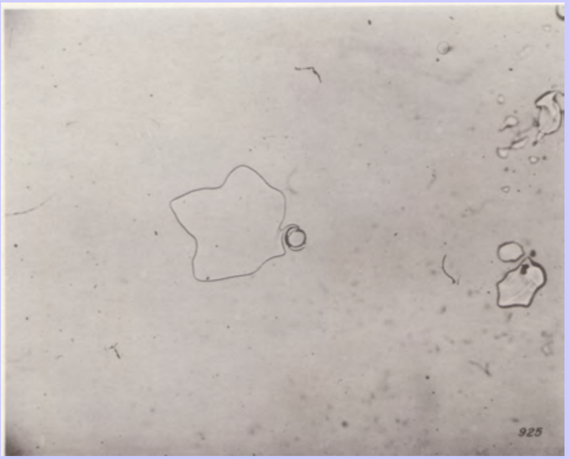


$t = 0$min.

$t = 3$min.



$t = 11$min.

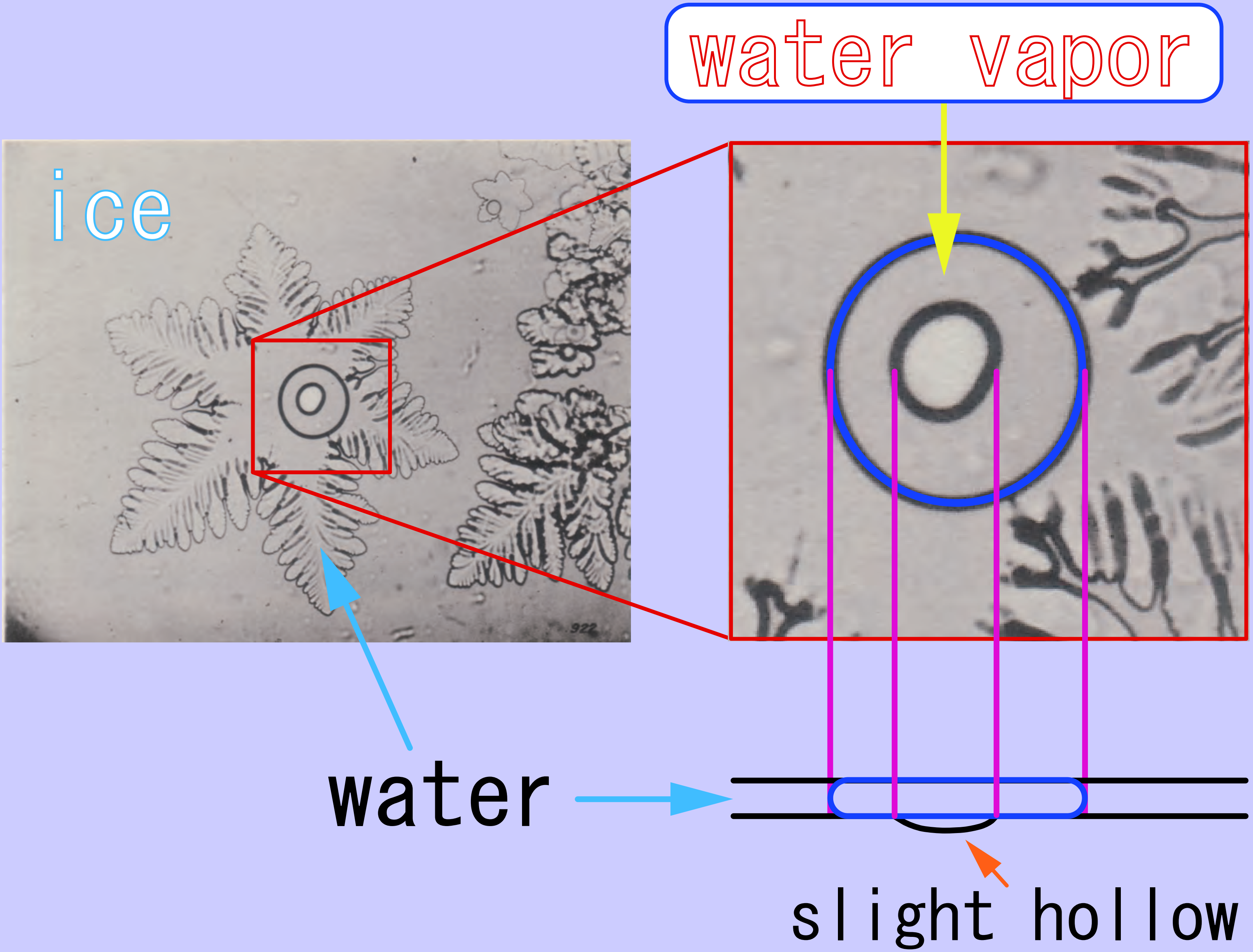


$t = 17$min.

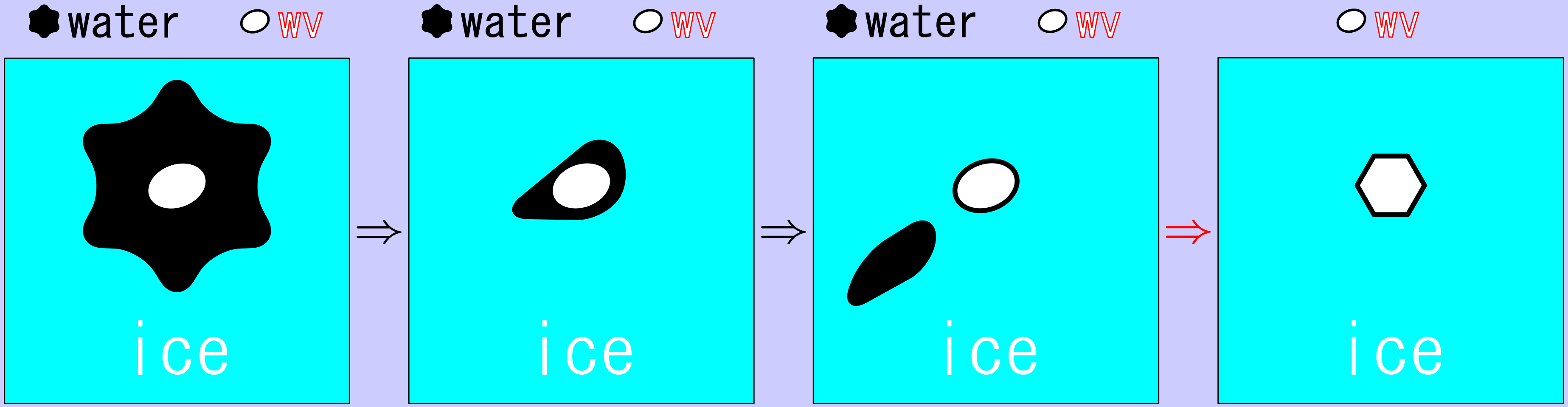
$t = 28$min.

$t = 1$hr 21min.

Remark



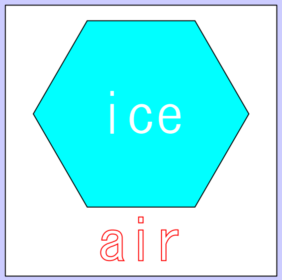
Negative crystal

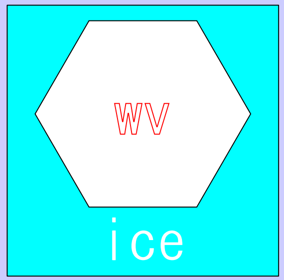


hexagonal disk

☆ McConnel found these disks
in the ice of Davos lake (1889).

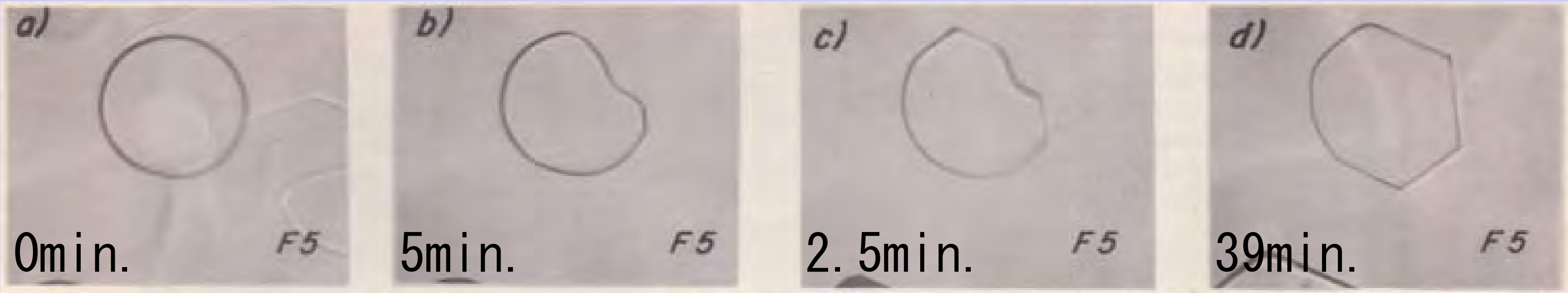
☆ Nakaya (1956) investigated its properties precisely.
He called the hexagon vapor figure.

the usual crystal: 

negative crystal: 

Observatin of the process “⇒”

Circle to Hexagon:



Nakaya’s observation:

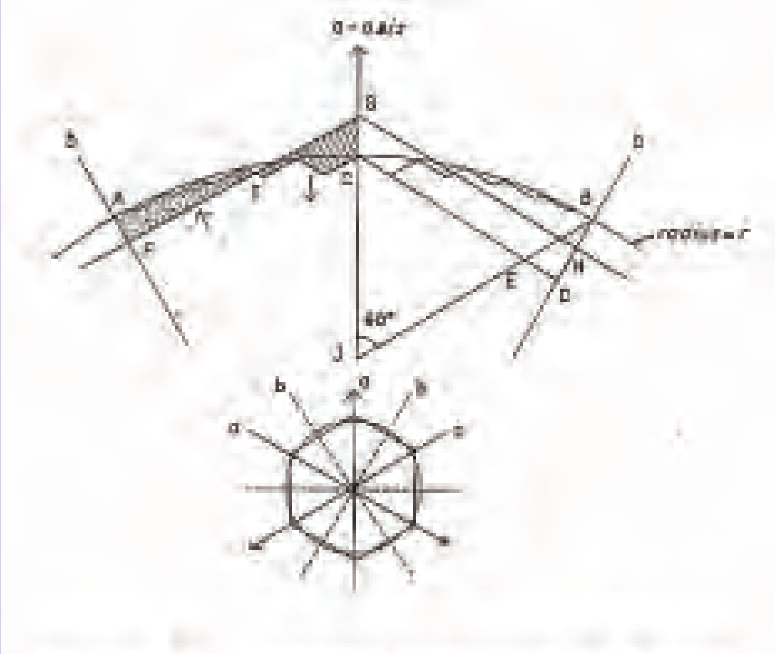
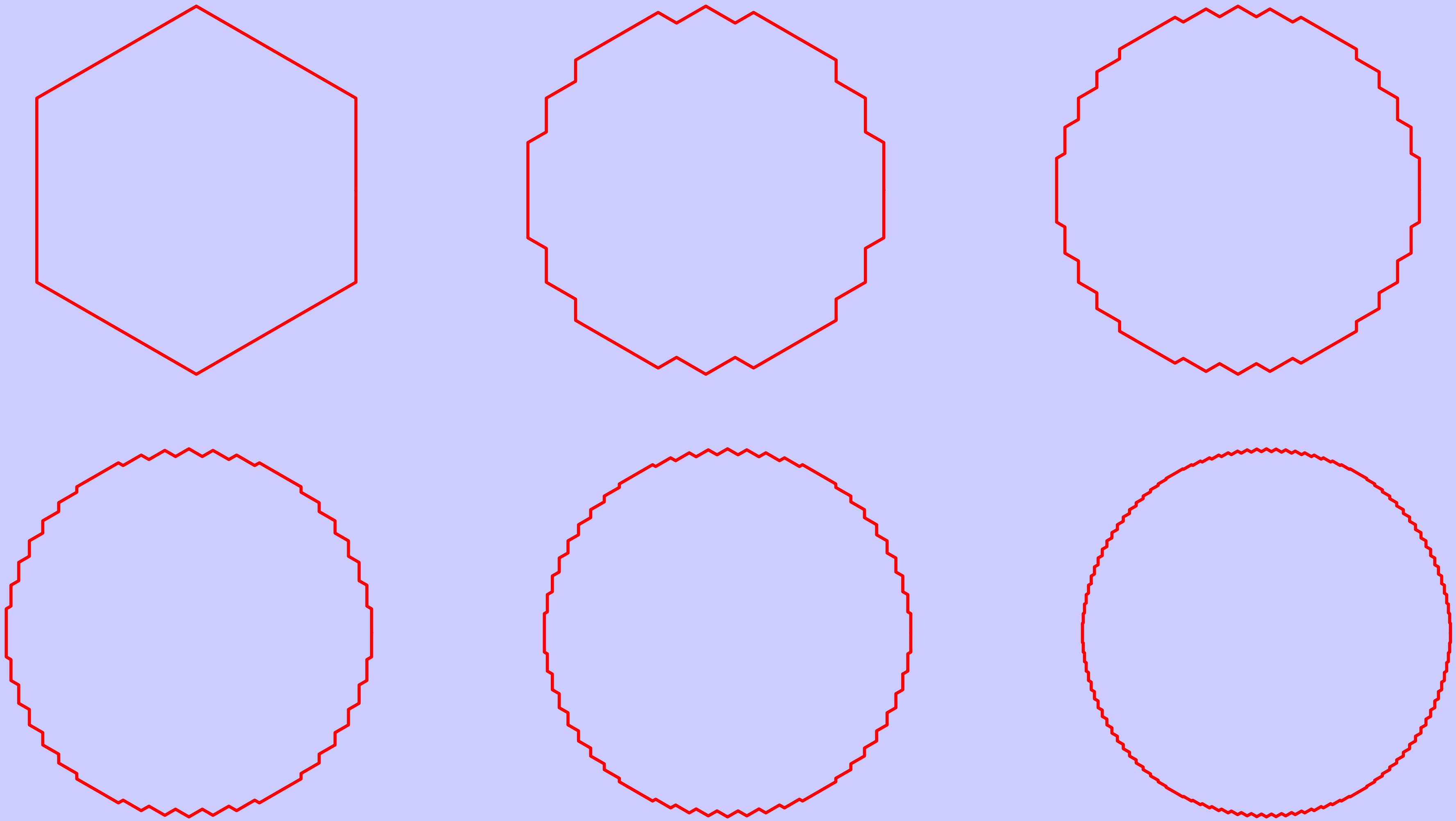


Figure 26. Stepped structure of the ice surface.

Stepped structure of the ice surface



Assumption and our model

Modeling the process "$\Rightarrow$" in the previous page

Ω: negative crystal (bdd in $\mathbb{R}^2$)

1) $\partial\Omega =$ moving curve

2) temperature $=$ a constant T:

(Ω is filled with water vapor saturated at T)

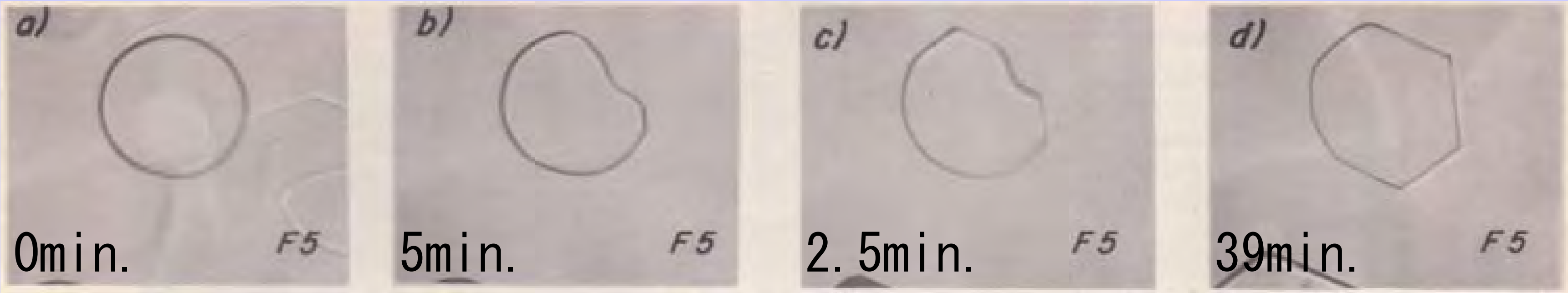
3) c-axis of the ice $\perp \mathbb{R}^2$

Our model a grad. flow of the interfacial energy:

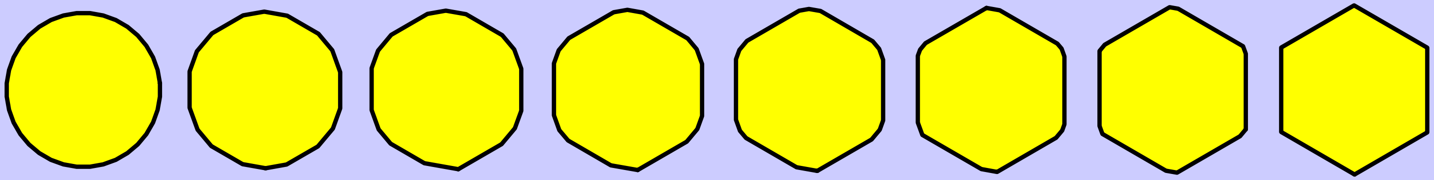
an Area-Preserving CCF equation

GOAL

Circle to Hexagon:



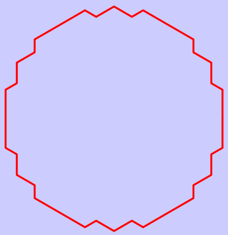
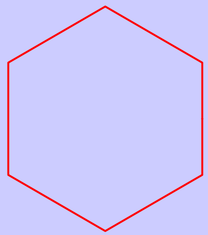
Goal 1: ess. adm. hexagon → hexagon (numerically)



movie

Goal 2: APCCF follows Nakaya's observation, i.e.

Thm.: almost convex hexagon

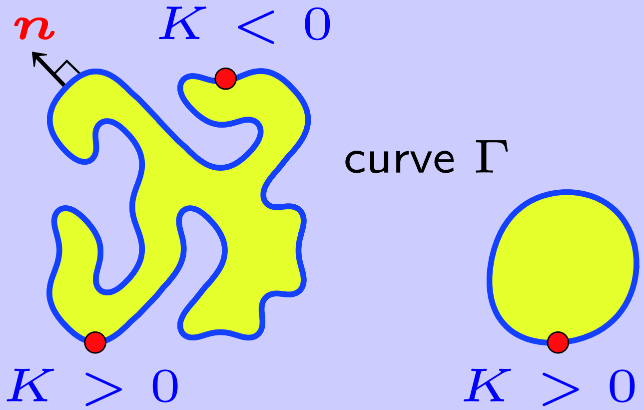
 converges to 

Curve-shortening / Area-preserving flow

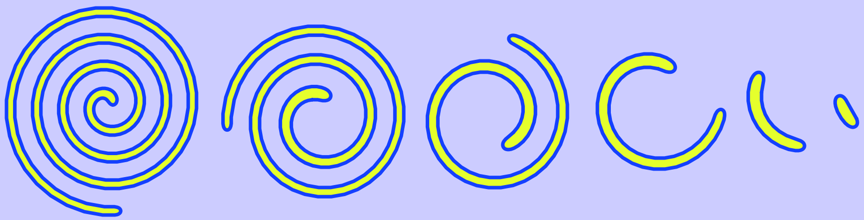
V: the normal velocity

$\boldsymbol{n}$: the outward unit normal vector

K: the curvature



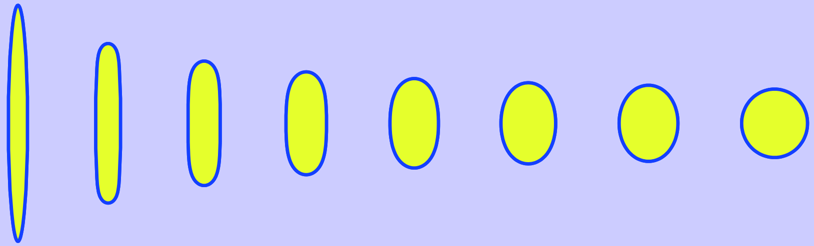
$$\boxed{V = -K}$$ . . Mullins('56), Brakke('78), Gage, Hamilton('86), Grayson('87), ...



$\Leftarrow$ Curve-shortening flow

movie

$$\boxed{V = \overline{K} - K}$$ ($\overline{K}$: average) . . . Gage('86), Mayer, Simonett(2000), ...



$\Leftarrow$ { Curve-shortening and
Area-preserving flow

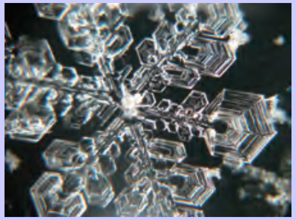
Anisotropy / Weighted curvature $K_\gamma(\boldsymbol{n})$

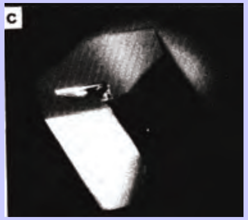
$K = \operatorname{grad} \mathcal{L} \cdot \boldsymbol{n}$, total length: $\mathcal{L} = \int_\Gamma ds$

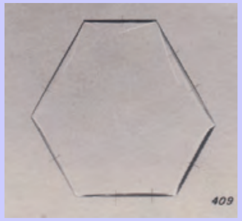
$V = \overline{K} - K$ $\Leftarrow$ $\operatorname{grad} \mathcal{L}$ flow subject to $\mathcal{A} \equiv const.$

Interfacial energy $\gamma(\boldsymbol{n})$

$\Leftarrow$ anisotropy







$K_\gamma(\boldsymbol{n}) = \operatorname{grad} \mathcal{E} \cdot \boldsymbol{n}$, total energy: $\mathcal{E} = \int_\Gamma \gamma(\boldsymbol{n})\, ds$

$$\boxed{V = \overline{K_\gamma} - K_\gamma(\boldsymbol{n})}$$

$\Leftarrow$ $\operatorname{grad} \mathcal{E}$ flow subject to $\mathcal{A} \equiv const.$

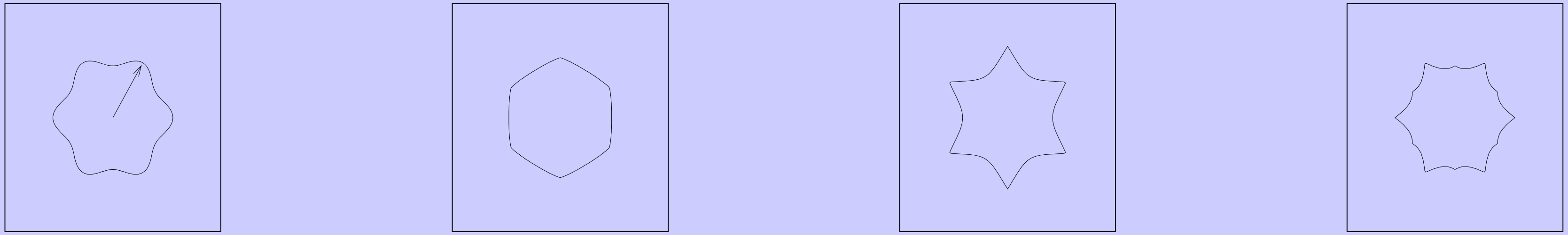
Question

If γ is not smooth,

what might happen to $\operatorname{grad}\mathcal{E}$?

Frank diagram $\mathcal{F}_\gamma$ / Wulff shape $\mathcal{W}_\gamma$

Frank diagram $\mathcal{F}_\gamma = \{\boldsymbol{n}/\gamma(\boldsymbol{n})\}$ $\Leftarrow$ Frank ('63), Meijering ('63)

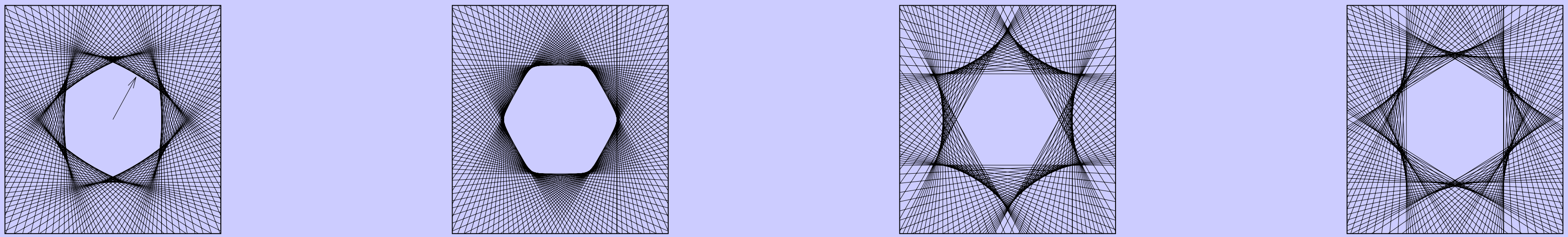


Wulff shape $\mathcal{W}_\gamma = \{\boldsymbol{x} \in \mathbb{R}^2 \,|\, \boldsymbol{x} \cdot \boldsymbol{n} \leq \gamma(\boldsymbol{n})\}$ $\Leftarrow$ the answer of

$\ll$ Wulff problem (on the equilibrium shape of crystals) $\gg$

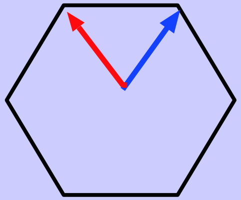
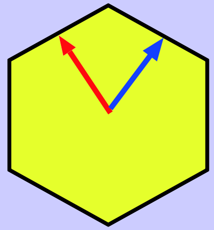
What is the shape which has the least $\mathcal{E}$ of the curve for the fixed enclosed area?

$\Leftarrow$ Gibbs (1878), Curie (1885), Wulff (1901)



Crystalline energy

γ is called crystalline energy

if $\mathcal{F}_\gamma$ is  $\Rightarrow \mathcal{W}_\gamma$: 

Weighted curvature flow $V = -K_\gamma(\boldsymbol{n})$

γ	$const.$	almost crystalline	almost crystalline
$\mathcal{W}_\gamma$	circle	round square	round hexagon
evolving graph	movie	movie	movie

γ: crystalline $\Rightarrow$ γ: non-differentiable $\Rightarrow$ $K_\gamma(\boldsymbol{n})$: not defined

Strategy by Taylor, and Angenent and Gurtin

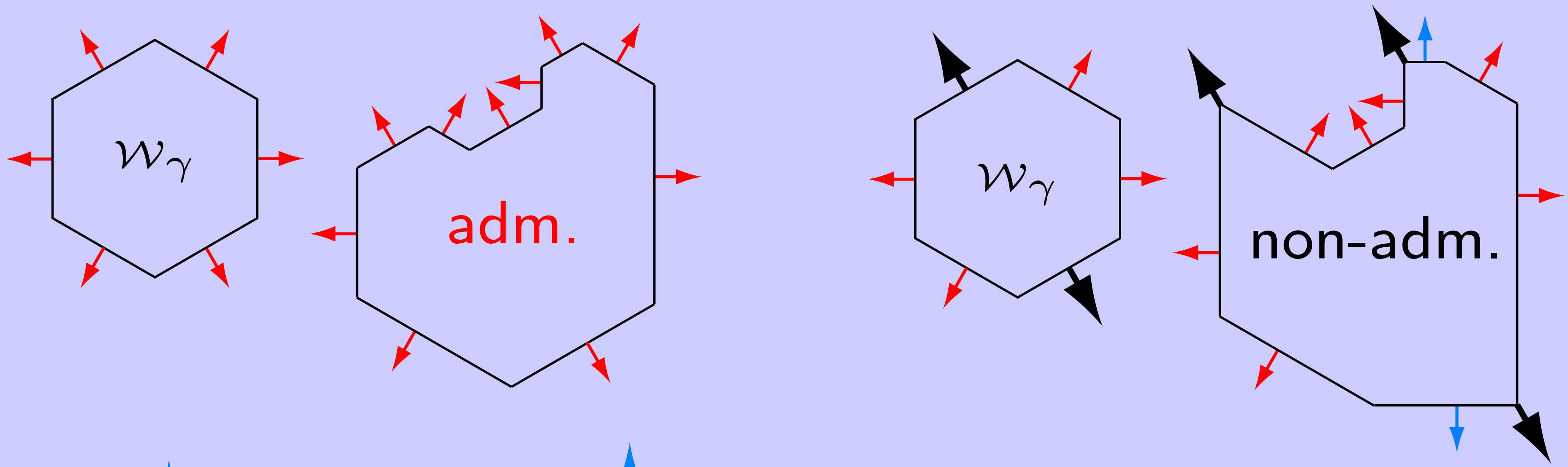
Γ: $y = u(x,t)$ $\quad \Rightarrow \mathcal{E} = \int_\Gamma \gamma \, ds = \int_0^1 g(u_x) \, dx$

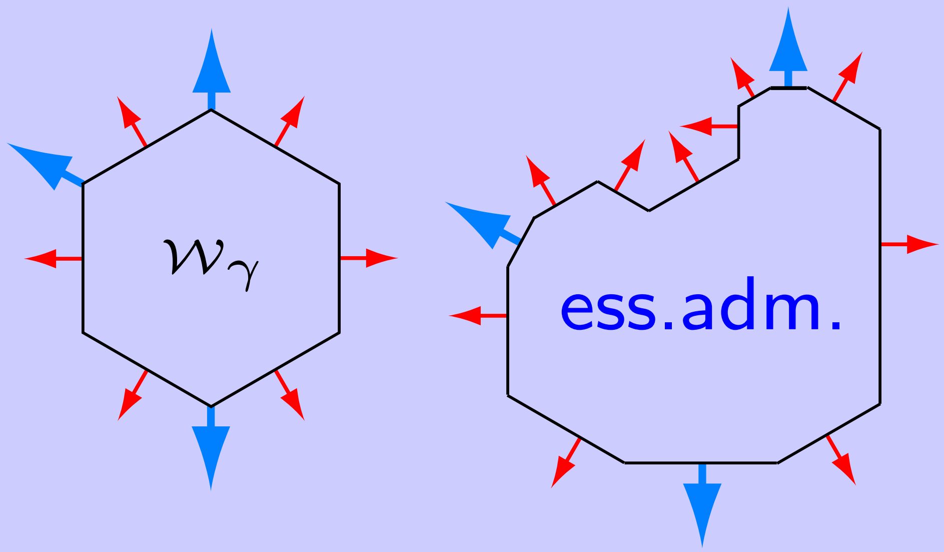
	$\gamma \equiv 1$	γ: smooth	$\mathcal{W}_\gamma$: square (γ is crystalline)
$g(u_x)$	$\mathrm{func}(u_x)$	$\mathrm{func}(u_x)$	$\lvert u_x \rvert + 1$
u_t	$\mathrm{func}(u_x) u_{xx}$	$\mathrm{func}(u_x) u_{xx}$	$\mathrm{func}(u_x)\delta(u_x) u_{xx}$
V	$-K$	$-K_\gamma(\boldsymbol{n})$	???

$\star$ Taylor and Angenent and Gurtin (in 1990 ± 1)

restrict Γ to an admissible class!

Admissible polygonal curve





Class of curves

admissible polygonal curves

$\Leftarrow$ Taylor ('90), Angenent, Gurtin ('89)

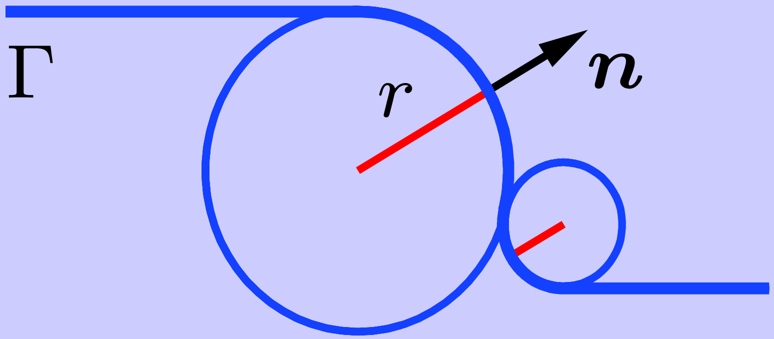
ess. adm. polygonal curves

$\Leftarrow$ Hontani, Giga, Giga, Deguchi (2005)

Area-preserving CCF

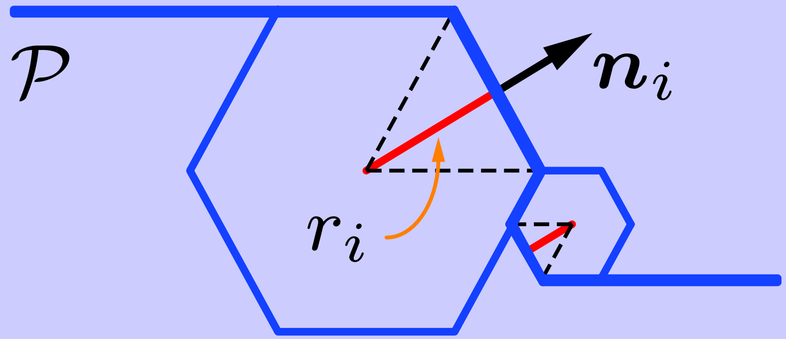
- Weighted curv. $= \mathrm{grad}_\Gamma \mathcal{E} = K_\gamma(\boldsymbol{n}) = w_\gamma(\boldsymbol{n})K$
- Crystalline curv. $= \mathrm{grad}_\mathcal{P} \mathcal{E} = K_\gamma(\boldsymbol{n}_i) = w_\gamma(\boldsymbol{n}_i)K_i$

$\star$ Case $\gamma \equiv 1$ and $\mathcal{W}_\gamma =$ a regular polygon:



the usual curvature

$K = \pm 1/r$



the crystalline curvature

$K_i = \pm 1/r_i$

$$V_i = \overline{K}_\gamma - K_\gamma(\boldsymbol{n}_i)$$

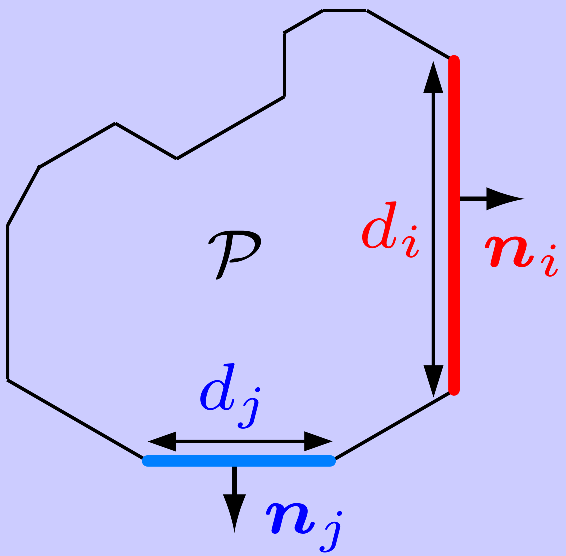
$\Leftarrow \mathrm{grad}_\mathcal{P} \mathcal{E}$ flow subject to $\mathcal{A} \equiv const.$

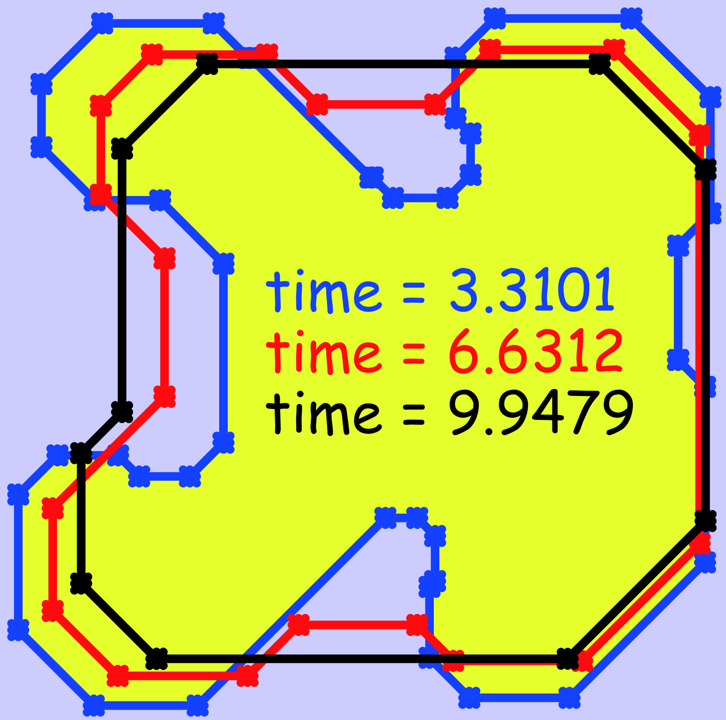
Problem (a sys. of ODEs): $\mathcal{P}(t) \to \,?\; (t \to T \le \infty)$

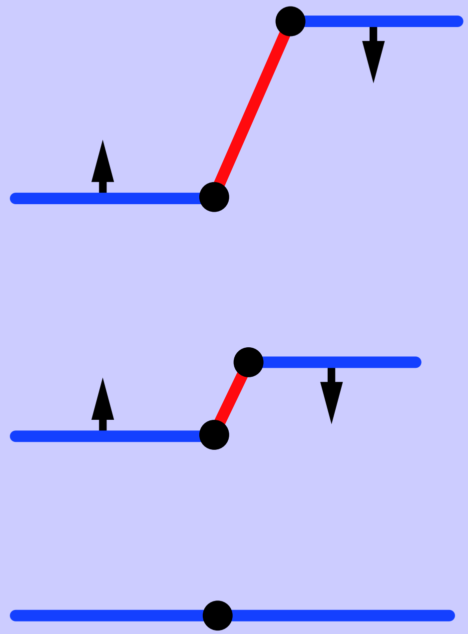
For a given (ess.) adm. curve $\mathcal{P}_0$ find a family of (ess.) adm. curves $\{P(t)\}_{0\le t<T}$ satisfying

$$\begin{cases} \dot{d}_i(t) = -(\cot\vartheta_i + \cot\vartheta_{i+1})V_i + \dfrac{V_{i-1}}{\sin\vartheta_i} + \dfrac{V_{i+1}}{\sin\vartheta_{i+1}} \quad (\forall i); \\ \mathcal{P}(0) = \mathcal{P}_0. \end{cases}$$

$$(\cos\vartheta_i = \langle \boldsymbol{n}_i, \boldsymbol{n}_{i-1} \rangle)$$





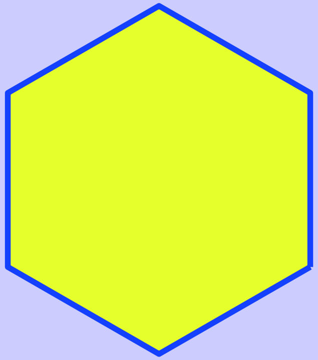


Case $\mathcal{P}_0$: admissible convex polygon

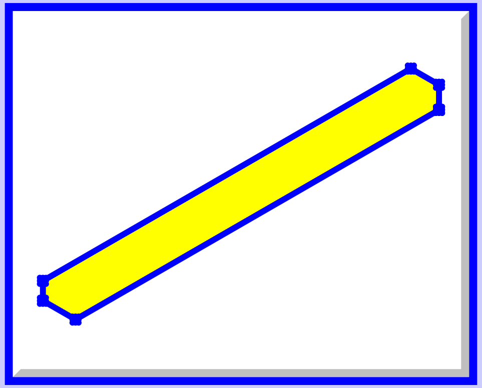
Isotropic case) $\gamma(\boldsymbol{n}_i) \equiv \gamma_*$ $(const.)$

Theorem (Yazaki (2002)): $\mathcal{P}(t) \to \mathcal{W}_{\gamma_*}$ as $t \to \infty$.

$\mathcal{W}_{\gamma_*}$:



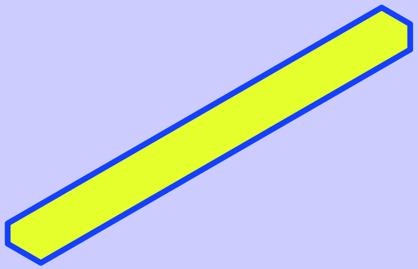
$\Longrightarrow$



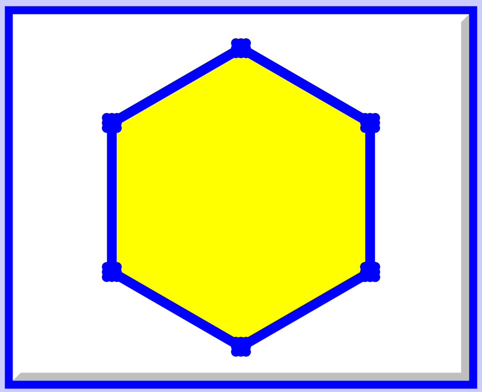
Anisotropic case) $\gamma(\boldsymbol{n}_i) \not\equiv const.$

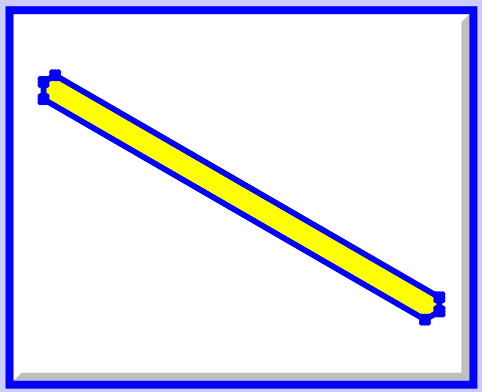
Theorem (Yazaki (2004)): $\mathcal{P}(t) \to \mathcal{W}_{\gamma}$ as $t \to \infty$.

$\mathcal{W}_{\gamma}$:



$\Longrightarrow$

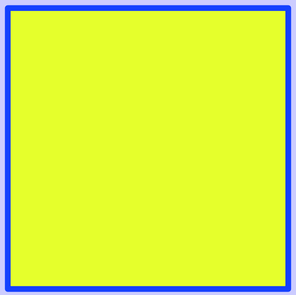
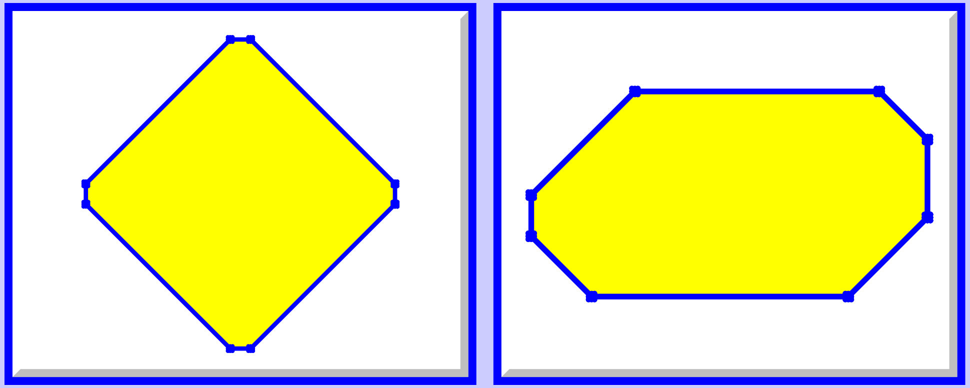




Case $\mathcal{P}_0$: ess. admissible convex polygon

Theorem (Yazaki): Let T be the max. exist. time.

If $T < \infty$, then $\inf_{0<t<T} \{\text{adm. edge } d_i(t)\} > 0$.

$\mathcal{W}_\gamma$:  $\Longrightarrow$ 

Open problems:

$T < \infty$ holds? for $\forall \mathcal{P}_0$: ess. adm. convex polygon

- If YES $\Rightarrow$ extension is possible:

  $\mathcal{P}_0 \to \mathcal{P}(T_1) \to \mathcal{P}(T_2) \to \cdots \to \mathcal{P}(T_m)$: adm.

  Note: YES in the case $V_i = g(\boldsymbol{n}_i, K_\gamma(\boldsymbol{n}_i), \overline{K}_\gamma)$

- If $\exists \mathcal{P}_0$ s.t. $T = \infty \Rightarrow \mathcal{P}(t) \to \mathcal{W}_\gamma$ as $t \to \infty$?

Case $\mathcal{P}_0$: adm. almost convex polygon

Ass. 1: anisotropic symmetry $\gamma(\boldsymbol{n}_i) = \gamma(-\boldsymbol{n}_i)$

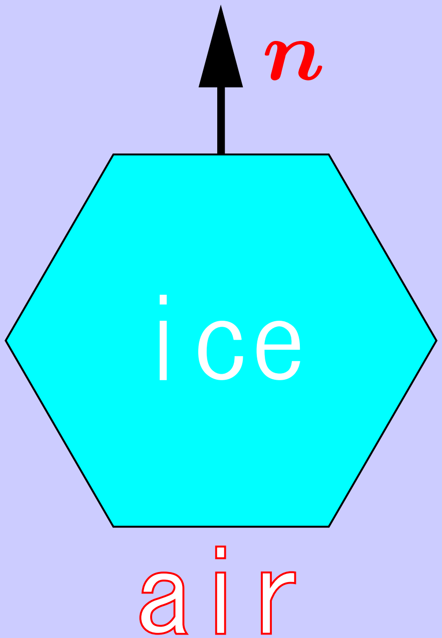
Ass. 2: $\mathcal{P}_0$ satisfies $K_\gamma(\boldsymbol{n}_i) \geq 0$ for all i.

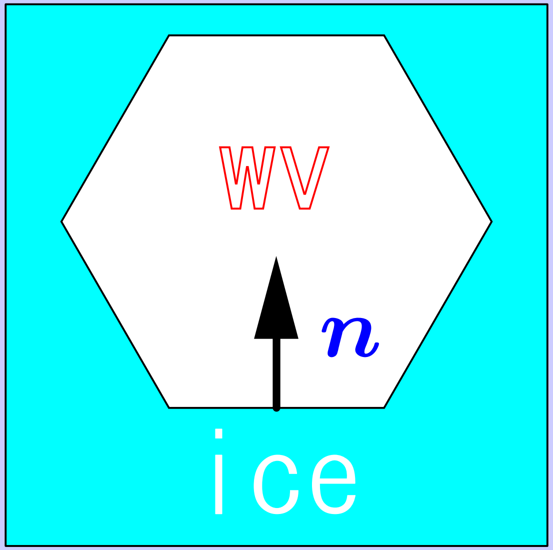
Theorem (Ishiwata-Yazaki):

$$\mathcal{P}_0 \to \mathcal{P}(T_1) \to \mathcal{P}(T_2) \to \cdots \to \mathcal{P}(T_m)\text{: adm.}$$

$\mathcal{P}(T_m)$ is admissible convex polygon.

APCCF: application to negative crystal



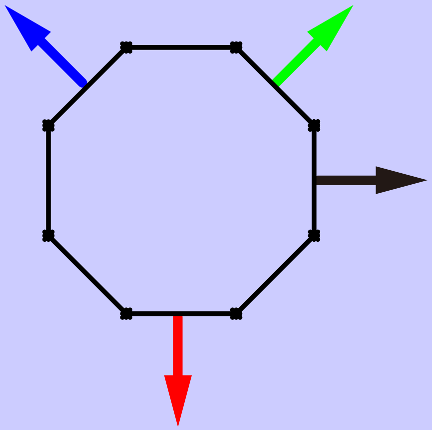


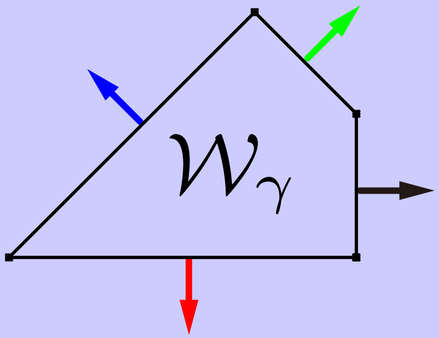
$\boldsymbol{n}$: outward normal
convex to $-\boldsymbol{n}$
$K_\gamma(\boldsymbol{n}) > 0$: positive
crystalline curv.

$\boldsymbol{n}$: outward normal
concave to $-\boldsymbol{n}$
$K_\gamma(\boldsymbol{n}) < 0$: negative
crystalline curv.

Anisotropy of negative crystal

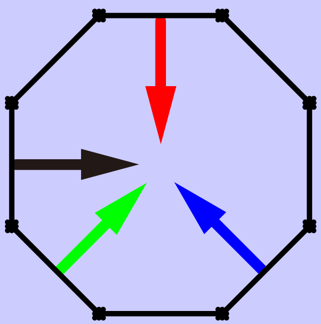
$\mathcal{W}_\gamma$-ess. admissible polygon $\mathcal{P}$:

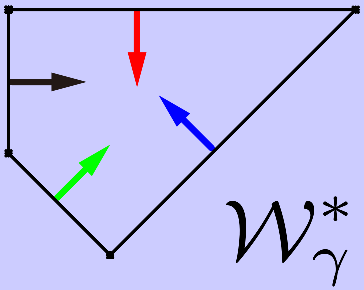




$$\mathcal{W}_\gamma = \bigcap_{j=1}^{J} \{ \boldsymbol{x} \in \mathbb{R}^2 ; \ \boldsymbol{x} \cdot \boldsymbol{\nu}_j \le \gamma(\boldsymbol{\nu}_j) \}$$

$\mathcal{W}_\gamma^*$-ess. admissible negative polygon $\mathcal{P}^*$:



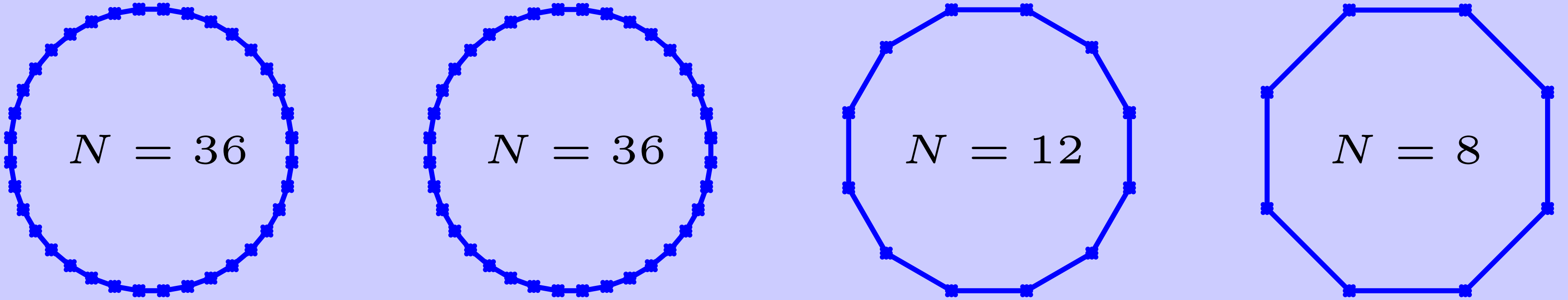


$$\mathcal{W}_\gamma^* = \bigcap_{j=1}^{J} \{ \boldsymbol{x} \in \mathbb{R}^2 ; \ \boldsymbol{x} \cdot (-\boldsymbol{\nu}_j) \le \gamma(\boldsymbol{\nu}_j) \}$$

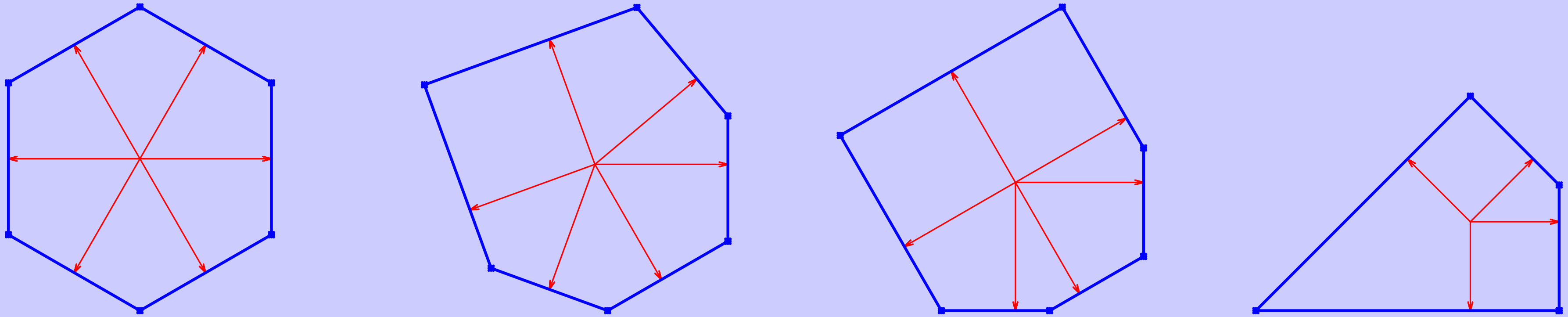
Remark: $\mathcal{W}_\gamma^* = \pi$-rot. of $\mathcal{W}_\gamma$

Simulation $\mathcal{P}^* \longrightarrow \mathcal{W}_\gamma^*$

the initial polygons are N-sided regular polygons:

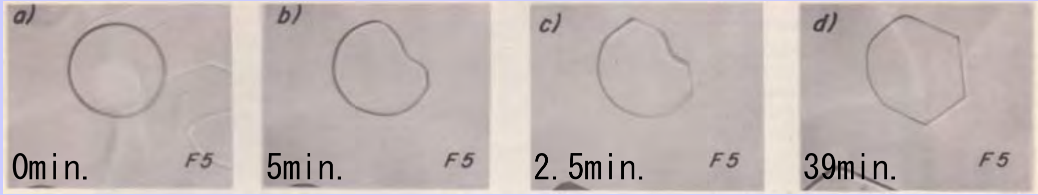


$\mathcal{W}_\gamma$'s are 6- or 4-sided polygons:



movie movie movie movie

Conclusion



Aim to track the motion of negative crystal Ω

Ass. 1: temperature is a constant T

Ass. 2: Ω is filled with water vapor saturated at T

Our model APCCF $V_i = \overline{K}_\gamma - K_\gamma(\boldsymbol{n}_i)$

Theorem: $\mathcal{W}_\gamma$-adm. almost convex $\mathcal{P} \to \mathcal{W}_\gamma$

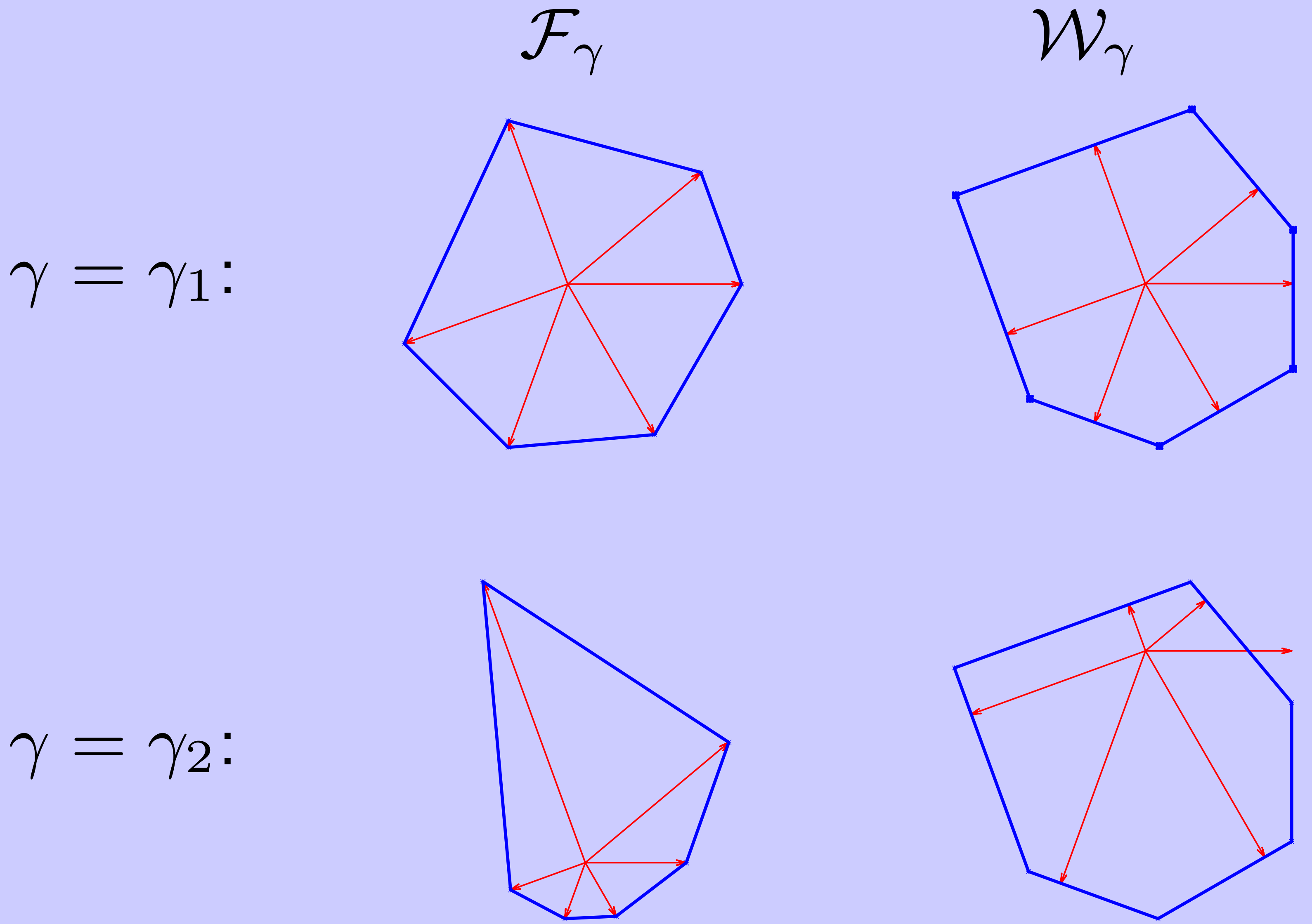
Application: $\mathcal{W}^*_\gamma$-adm. almost convex $\mathcal{P}^* \to \mathcal{W}^*_\gamma$

Simulation: $\mathcal{W}^*_\gamma$-ess. adm. $\mathcal{P}^* \to \mathcal{W}^*_\gamma$

Future research to remove the Ass. 1.

$\Rightarrow$ Ω is filled with super- or sub-saturated water vapor, depending on the position.

There exist $\gamma_1 \neq \gamma_2$ s.t. $\mathcal{W}_{\gamma_1} = \mathcal{W}_{\gamma_2}$:



Numerical scheme

ODEs:

$$\dot{d}_i(t) = -(\cot\vartheta_i + \cot\vartheta_{i+1})V_i + \frac{V_{i-1}}{\sin\vartheta_i} + \frac{V_{i+1}}{\sin\vartheta_{i+1}} \ (\forall i)$$

- (1) $\dot{\mathcal{E}}(t) \le 0$; (2) $\dot{\mathcal{A}}(t) = 0$.

Numerical scheme:

$$\left((D_\tau f)^m = \frac{f^{m+1} - f^m}{\tau_m} \right)$$

$$(D_\tau d_i)^m = -(\cot\vartheta_i + \cot\vartheta_{i+1})V_i^{m+\mu} + \frac{V_{i-1}^{m+\mu}}{\sin\vartheta_i} + \frac{V_{i+1}^{m+\mu}}{\sin\vartheta_{i+1}}$$

- $\mu \in (0,1]$: implicit scheme $\Rightarrow$ solved by iteration
- (1) $(D_\tau\mathcal{F})^m \le 0 \ (\forall\mu)$; (2) $(D_\tau\mathcal{A})^m = 0 \ (\mu = 1/2)$.