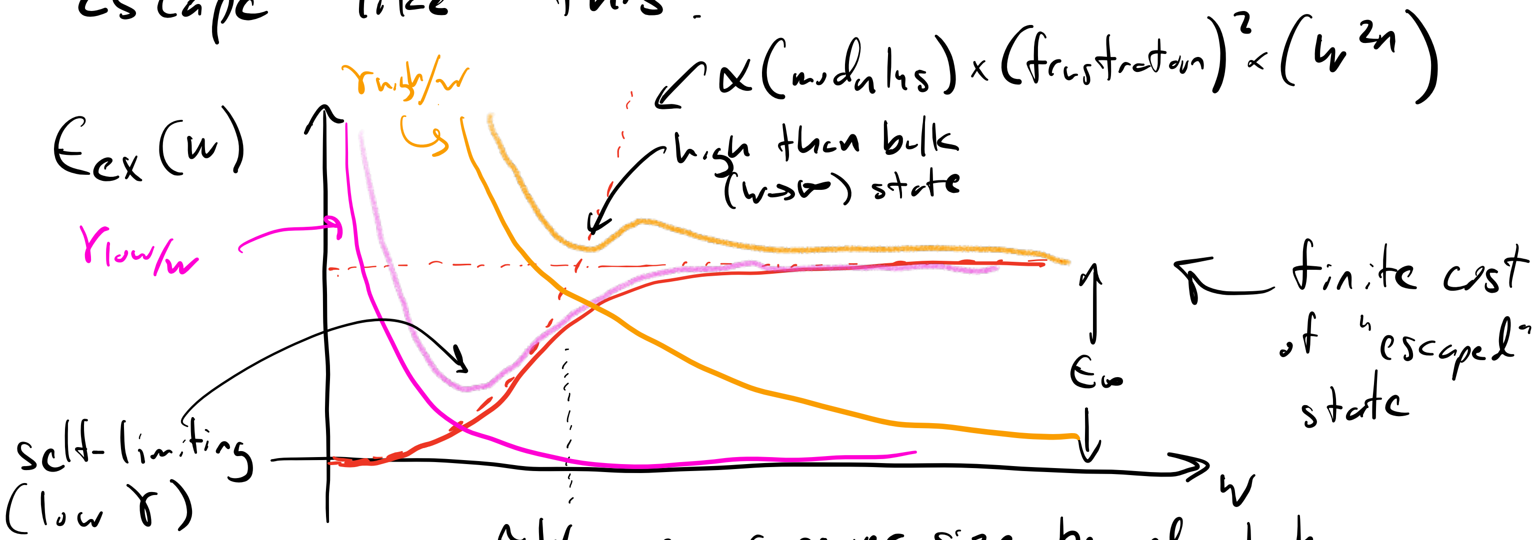
IV Mechanisms of frustration escape

We have previously seen how superextensive elastic cost of frustration leads to self-limiting domain selection.

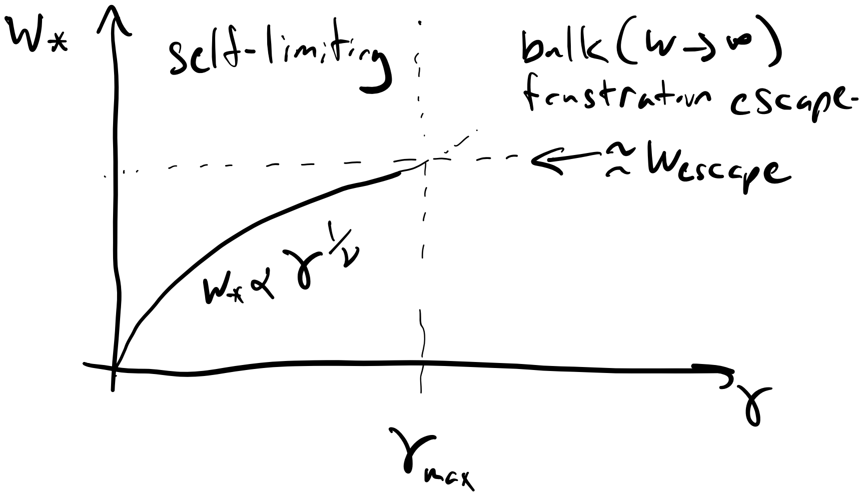
Here we consider mechanisms of "frustration escape", where at some sufficiently large scale, some finite energy density motif becomes accessible, leading to extensivity at large size.

Schematically, picture thermodynamics of escape like this:



$\simeq W_{escape}$, crossover size beyond which frustration can be absorbed into higher energy state

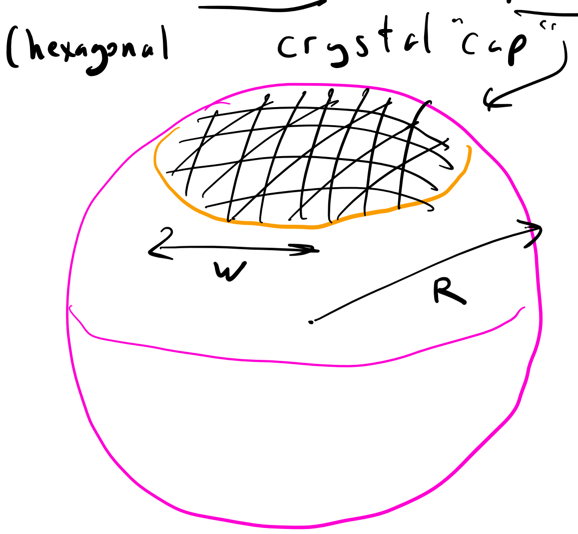
Based on this sketch, we expect bulk (frustration escape) for large enough γ



Here, we'll discuss 2 competing "modes" of frustration escape

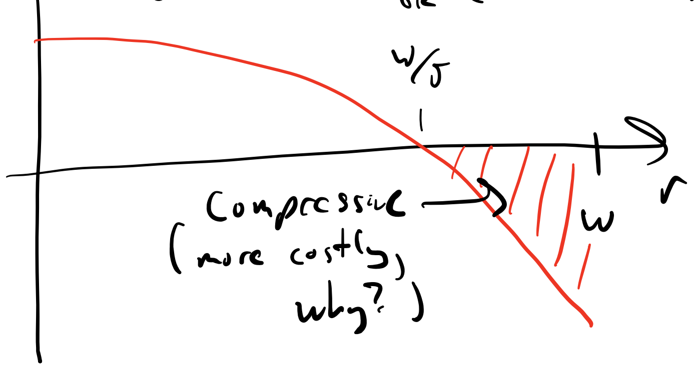
- Topological defects
- "Shape flattening"

Ex. Defects in spherical crystals (Li, Zandi, Travesset, Grason, PRL 2019)

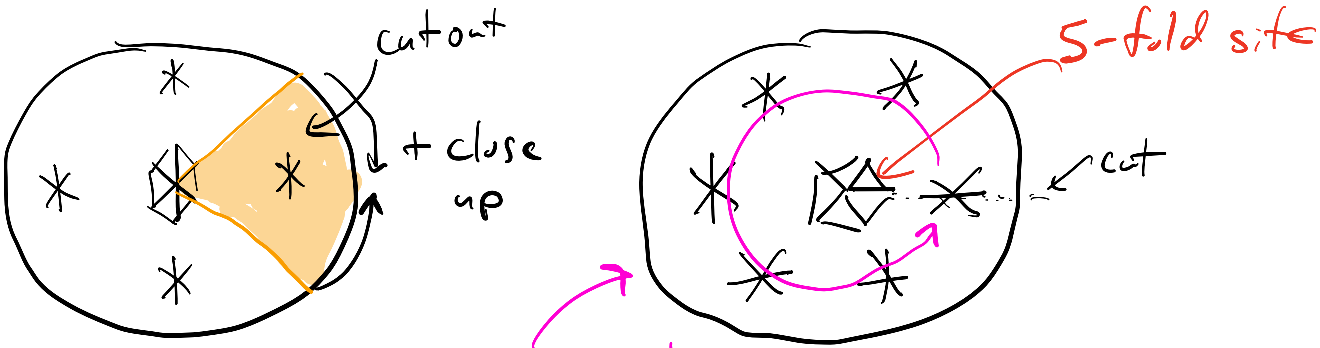


Recall gradient stress

$$\sigma_{K_G} = \sigma_{\phi\phi} + \sigma_{rr} = \frac{Y}{8R^2}(w^2 - 2r^2)$$



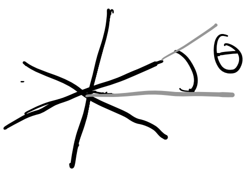
One way to mitigate cost of outer compression is to remove material (Volterra cut)



crystal directors rotate by $+\frac{2\pi}{6}$ = disclination

orientation defect

See e.g. Seung & Nelson, PRA 1988

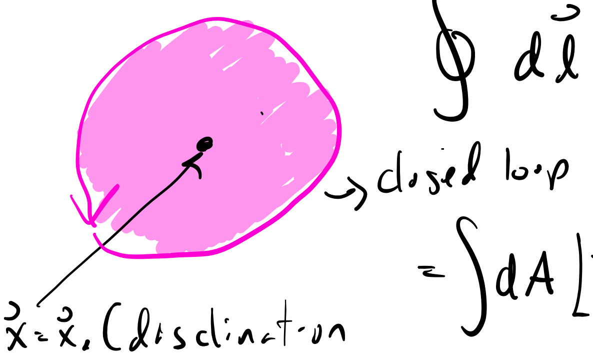


$$\theta(\vec{x}) \simeq \frac{1}{2}(\partial_x u_y - \partial_y u_x)$$

"charge"

$$\oint d\vec{l} \cdot \nabla\theta = s = n\left(\frac{2\pi}{6}\right)$$

integer



$$= \int dA \left[\nabla_\perp \times (\nabla_\perp \theta)\right]$$

$n = +1 \Rightarrow$ 5-fold

$n = -1 \Rightarrow$ 7-fold

$$\nabla_\perp \times (\nabla_\perp \theta) = s\,\delta(\vec{x} - \vec{x}_0)$$ charge density

$\frac{\epsilon_{ij}}{2} \partial_i u_j$

Because derivatives don't commute $(\partial_x \partial_y \theta \neq \partial_y \partial_x \theta)$ at defect, this modifies compatibility

$$\partial_x^2 \varepsilon_{yy} + \partial_y^2 \varepsilon_{xx} - 2\partial_x \partial_y \varepsilon_{xy} = s\,\delta(\vec{x} - \vec{x}_0) - K_G$$

Modified Foppl-van Karman

$$\frac{1}{Y}\nabla_\perp^2 \sigma_{kk} = \sum_i s_i\, \delta(\vec{x}-\vec{x}_i) - K_G$$

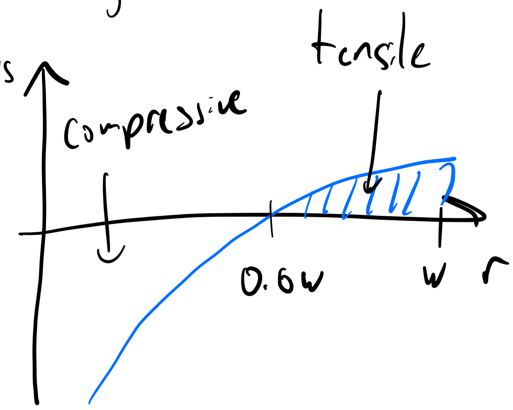
smooth, background source

point-like source

Solve $\frac{1}{Y}\nabla_\perp^2 \sigma = s\,\delta(\vec{r})$ + B.C. + $\partial_i \sigma_{ij} = 0$

(Grason, PRE 2012)

$$\Rightarrow \sigma_{dis} = \frac{Ys}{2\pi}\left[\ln\left(\frac{r}{w}\right)+\frac{1}{2}\right]$$



Elastic energy (superposition)

$$\sigma = \sigma_{K_G} + \sigma_{dis}\left(s = \tfrac{2\pi}{6}n\right) \Rightarrow E \approx \frac{1}{Y}\int dA\,(\sigma)^2$$

$$\frac{E_{TOT}}{Y(\text{Area})} = \frac{1}{384}\left(\frac{W}{R}\right)^4 + \frac{n^2}{288} + \cancel{E_{core}} - \frac{n}{192}\left(\frac{W}{R}\right)^2$$

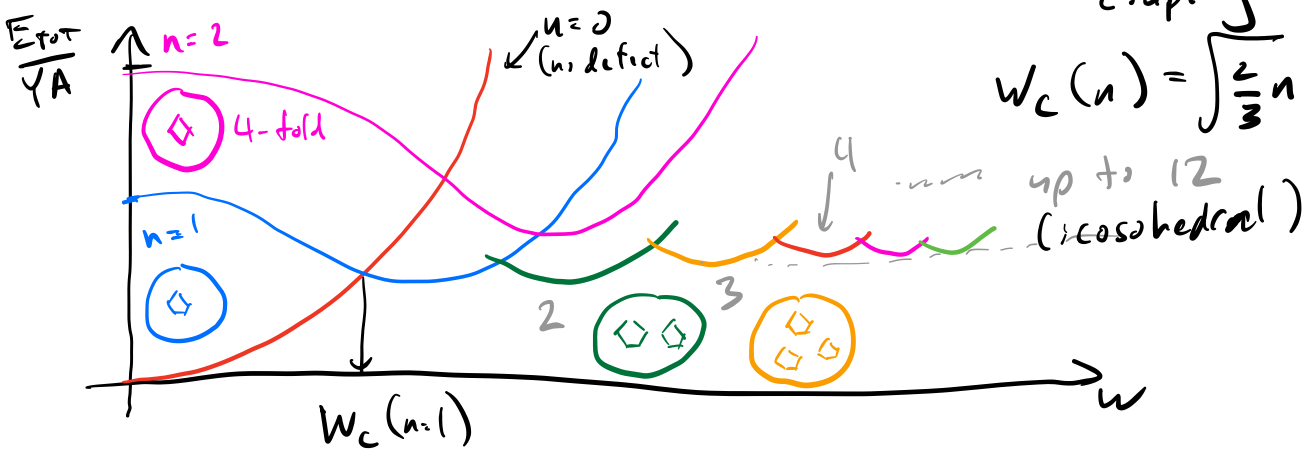
ignore

frustration

self-energy (defect)

curvature / defect coupling

$$W_c(n) = \sqrt{\frac{2}{3}n}\,R$$



Here, escape is discontinuous sequence of 1st order transitions between defect #.

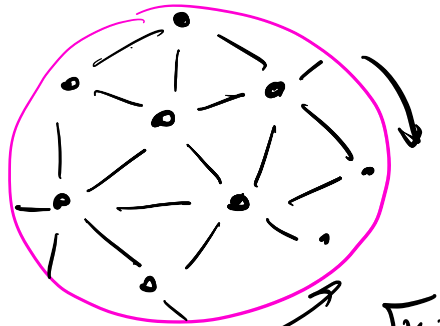
At large size, expect "perfect screening"

$$\int dA \left(\sum_i s_i \, \delta(\vec{x} - \vec{\alpha}_i) - K_G \right) = 0$$

$$s_0 \rho_d - K_G$$

areal defect density

$$\rho_d = \frac{K_G}{s_0} \propto \frac{1}{l_d^2}$$



$l_d \propto \sqrt{K_G^{-1}} = R$

Up to this point, we have assumed magnitude of frustration (K_G) is fixed.

But in many assemblies, there is finite elastic cost to "deform frustration", leading to a distinct mode of elastic "shape flattening" to escape frustration

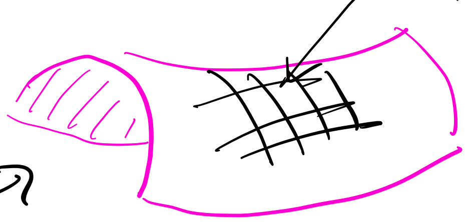
Here, we consider a model previously introduced by (M. Moshe lectures)

Ex. Hyperbolic membrane assemblies

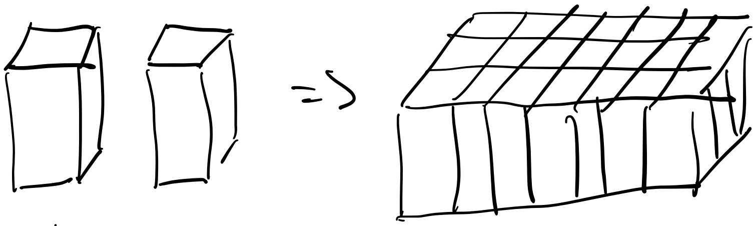
(Armon et al. Soft Matter 2014, Ghafouri & Bruinsma, PRL 2005, Hall et al., Soft Matter 2023)

+ "flat" 2D crystalline order (favored)

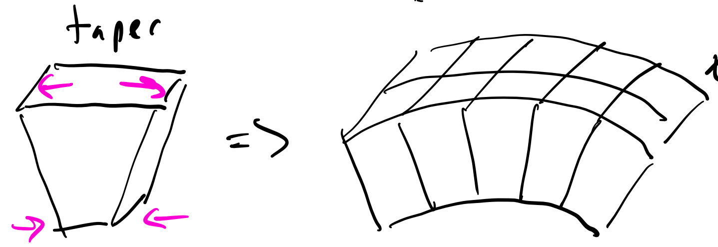
locally favored saddle shape



Molecular Building Blocks

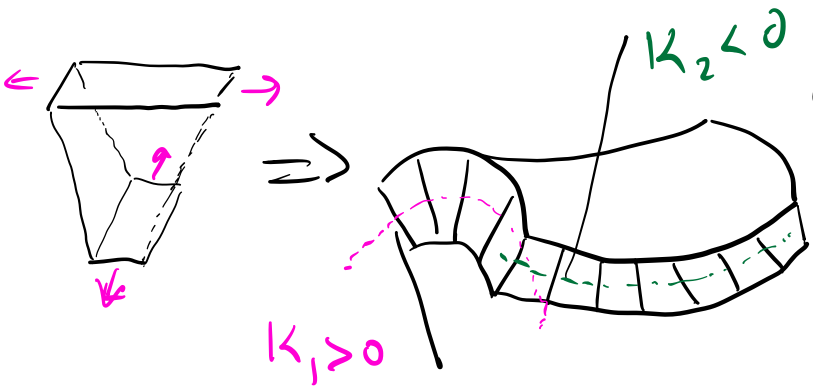


flat crystalline membrane.



preferred curvature K_0

"double taper"



preferred saddle

Incompatible elasticity (small slopes)

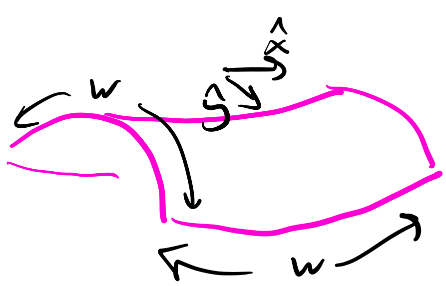
$$E_{elas} = \int dA \left[\frac{1}{2} \varepsilon_{ij} \sigma_{ij} + \frac{B}{2} \left(K_{ij} - K_{ij}^{0} \right)^2 \right]$$

cost for "non-flat" metric

bending cost from preferred shape

K_{ij} = curvature tensor

Assume square boundary



$$K^{0} = \begin{pmatrix} K_{\parallel}^{0} & 0 \\ 0 & -K_{\perp}^{0} \end{pmatrix}$$

Crude approximation (thick sheet small w).

$\Rightarrow$ spatially uniform K_x, K_y $\quad K_G = K_x K_y$

$$\int dA \, \tfrac{1}{2} \varepsilon_{ij} \sigma_{ij} \cong \underbrace{c_0}_{\text{const. (depends of domain shape)}} Y K_G^2 w^4 \, (\text{Area})$$

$$\frac{E_{elas}}{\text{Area}} \cong c_0 Y w^4 (K_x K_y)^2 + B\left[(K_x - K_{\parallel}^0)^2 + (K_y + K_{\perp}^0)^2\right]$$

only frustrated when K_x & $K_y \neq 0$

Consider limits

$w \to 0$ (frustration cost $\ll$ bending)

$\Rightarrow K_x = -K_{\parallel}^0$; $K_y = K_{\perp}^0$ (favored shape)

$$\frac{E_{elas}}{\text{Area}} \simeq Y w^4 (K_{\perp}^0 K_{\parallel}^0)^2 + \underline{\text{no bending cost}}$$

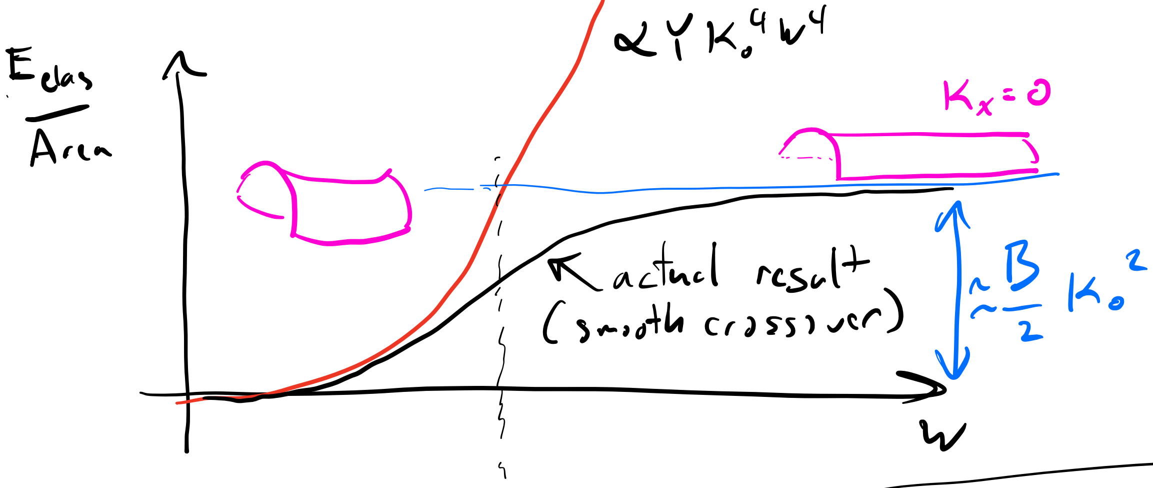
$w \to$ large (frustration cost $\gg$ bending)

Expect $K_x K_y \to 0$ (shape flattening)

$$\text{either} \begin{cases} K_x = 0 & K_y = -K_{\perp}^0 \\ K_x = K_{\perp}^0 & K_y = 0 \end{cases}$$

$$\frac{E}{\text{Area}} = \frac{E_{flat}}{\text{Area}} \simeq \frac{B}{2} K_0^2$$

* only needs to flatten along 1 of two directions



$$Y K_0^4 w_{flat}^4 \approx \frac{B}{2} K_0^2 \Rightarrow \boxed{w_{flat} \approx \left(\frac{B}{Y} K_0^{-2} \right)^{1/4}}$$

Notice that $\sqrt{\frac{B}{Y}} \equiv t$ elastic thickness (expect this to be ~ subunit size)

$w_{flat} \approx \sqrt{t\, K_G^{-1/2}}$ ← smooth, elastic flattening

$w_{dis} \approx \sqrt{|K_G|^{-1}}$ ← size for stable disclinations

Note that $\frac{w_{flat}}{w_{dis}} \approx \sqrt{\frac{t}{K_G^{-1/2}}} \ll 1$ for small subunits

Hence for this example, we expect smooth shape flattening to preempt defect formation and set the upper limit to superextensivity (SLA)