Topological Defects

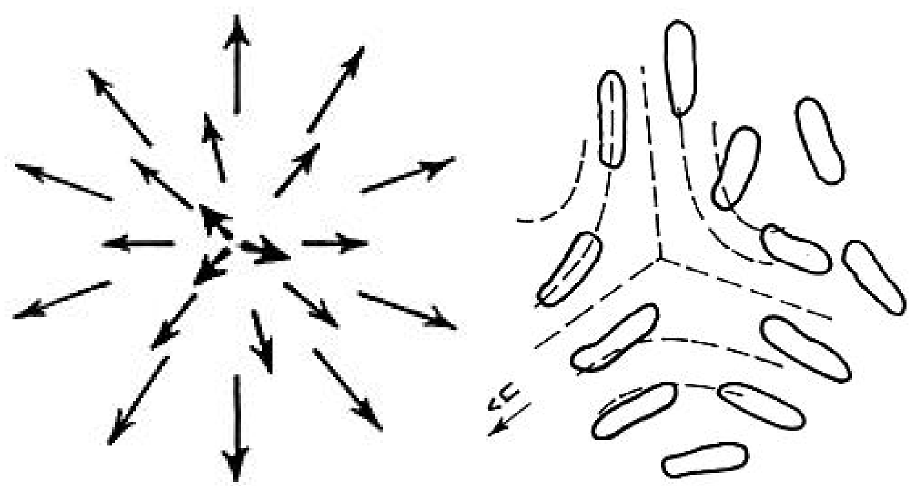
18.S995 - L23

Order Parameters, Broken Symmetry, and Topology

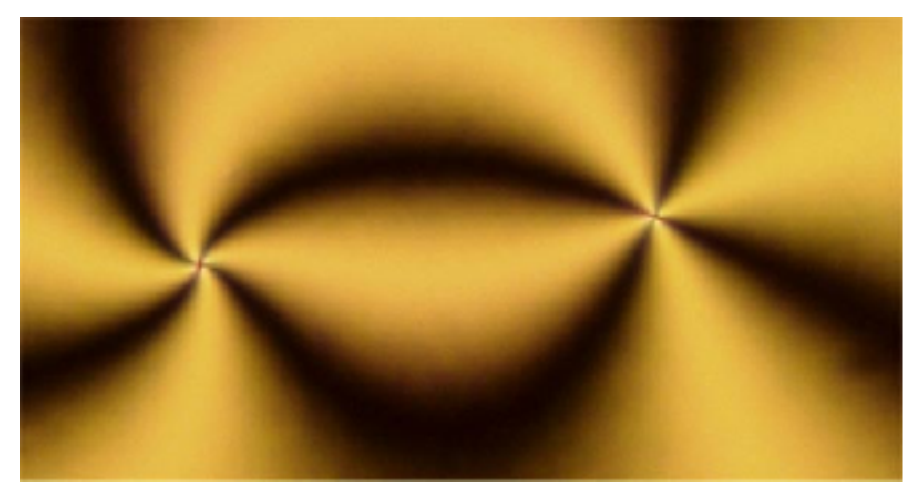
James P. Sethna
Laboratory of Applied Physics, Technical University of Denmark,
DK-2800 Lyngby, DENMARK, and NORDITA, DK-2100 Copenhagen Ø,
DENMARK and Laboratory of Atomic and Solid State Physics (LASSP),
Clark Hall, Cornell University, Ithaca, NY 14853-2501, USA
(Dated: May 27, 2003, 10:27 pm)

dunkel@mit.edu

Topological defects are discontinuities in order-parameter fields



- optical effects
- work hardening, etc

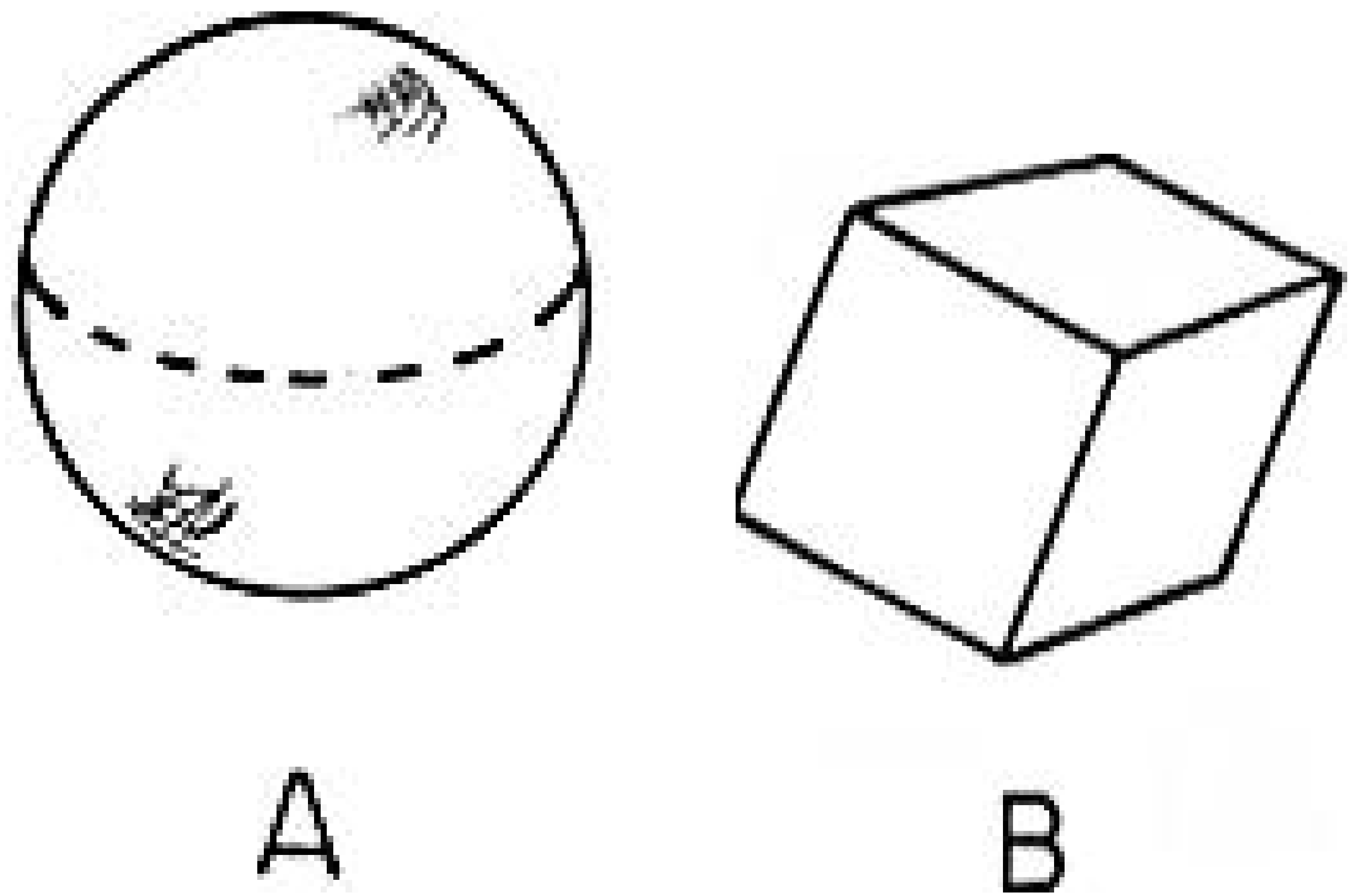


"umbilic defects" in a nematic liquid crystal order = symmetry = invariance

(under certain group actions)

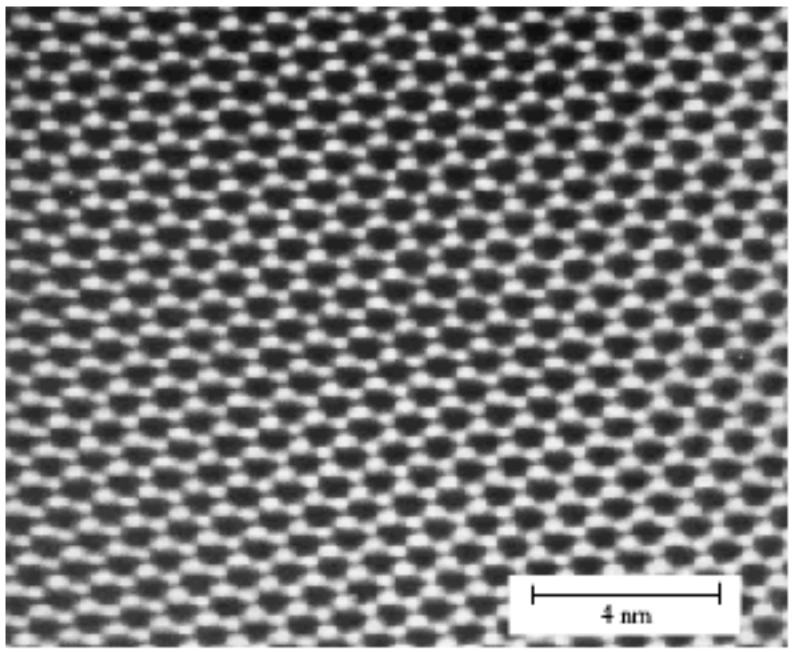
symmetry groups can be discrete,
continuous, Lie-groups, ….

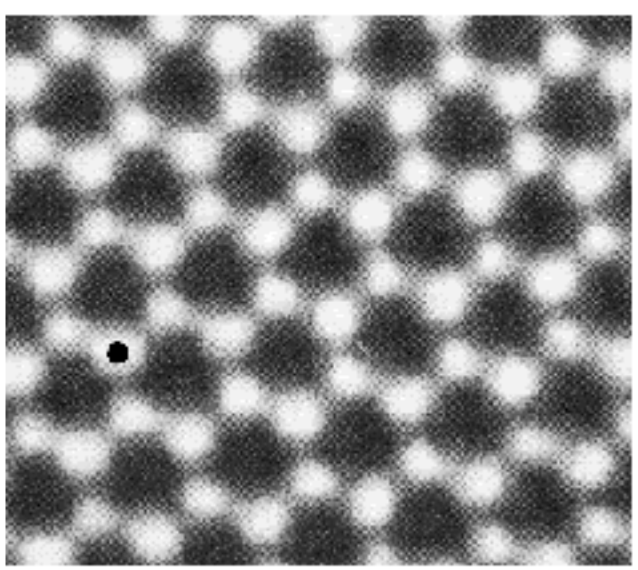
More or less symmetric ?

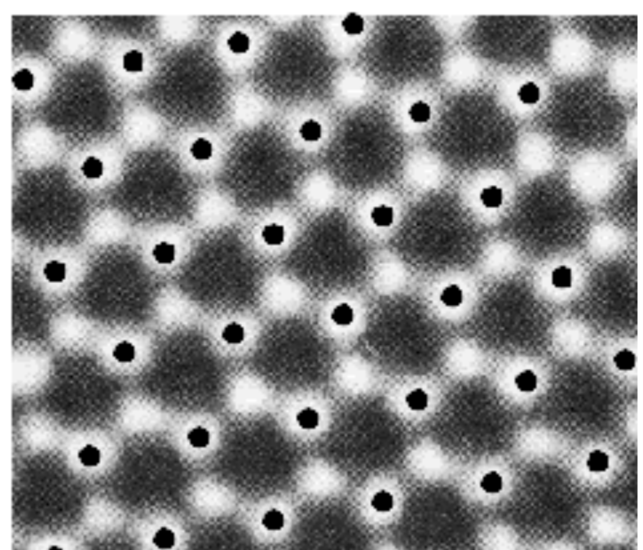


More or less symmetric ?

$Mg_2Al_4Si_5O_{18}$

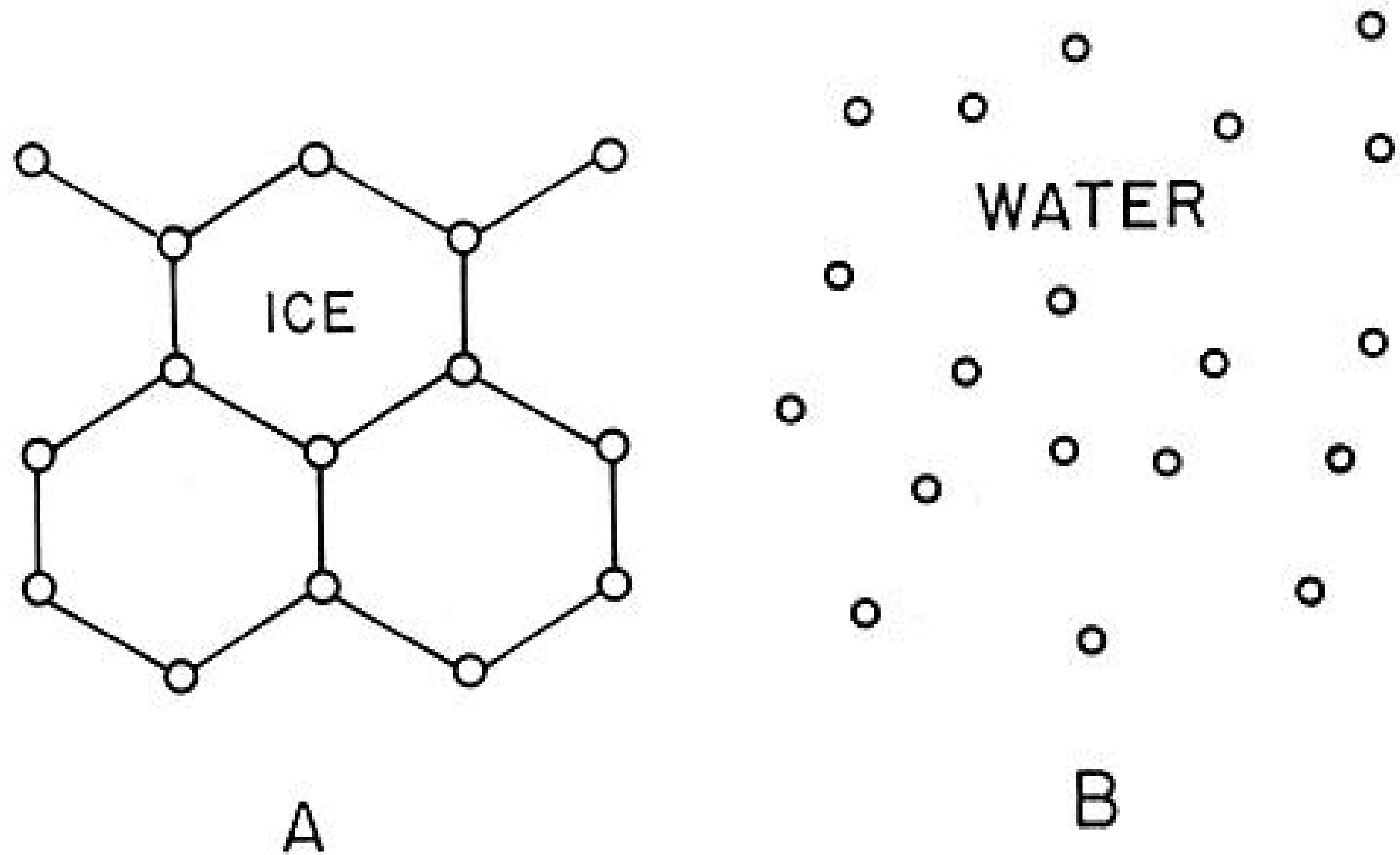






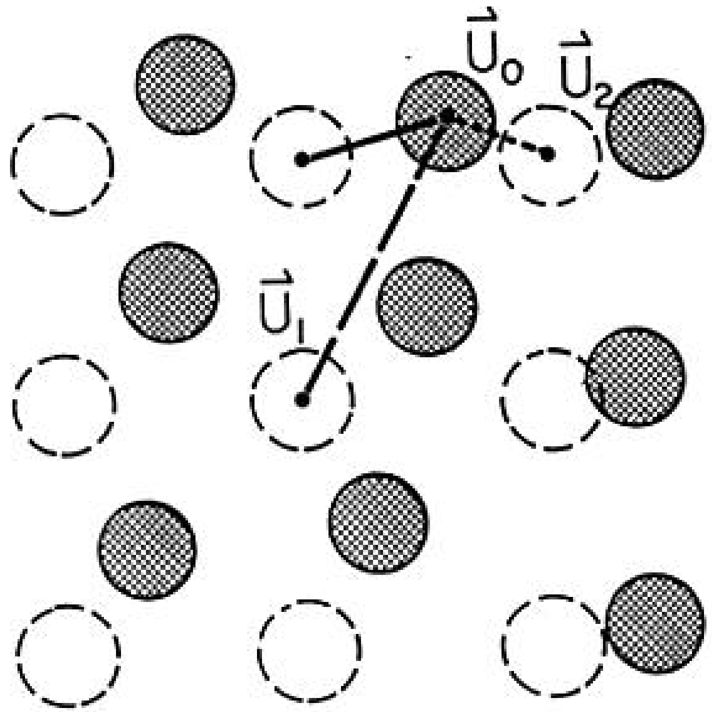
http://www.doitpoms.ac.uk/tlplib/crystallography3/printall.php

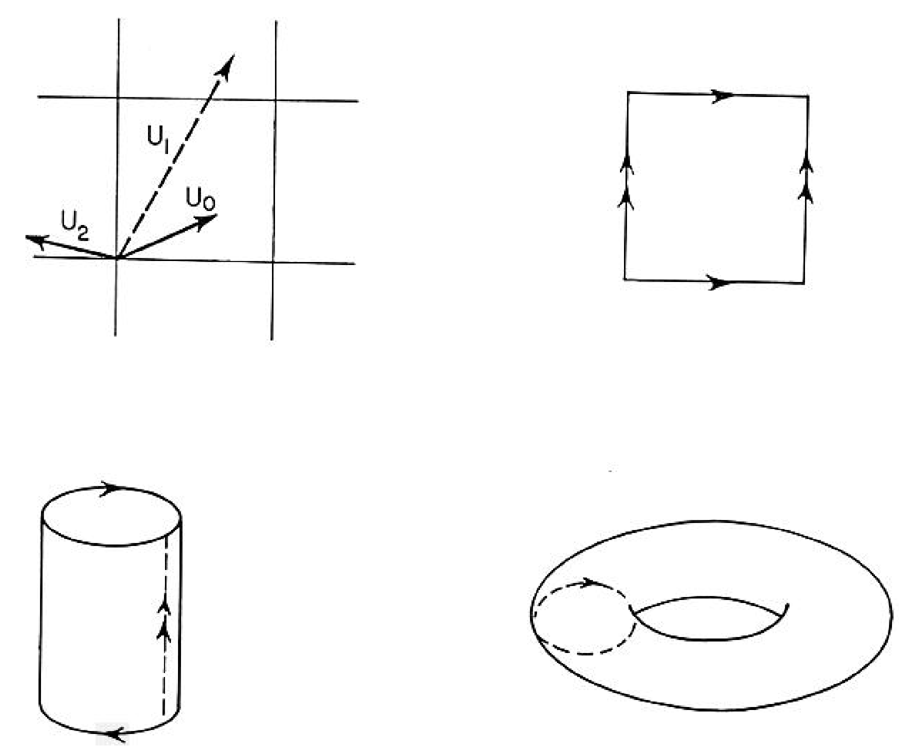
More or less symmetric ?



broken continuous
translation/rotation
symmetry (invariance)

Order parameters:
2D crystal

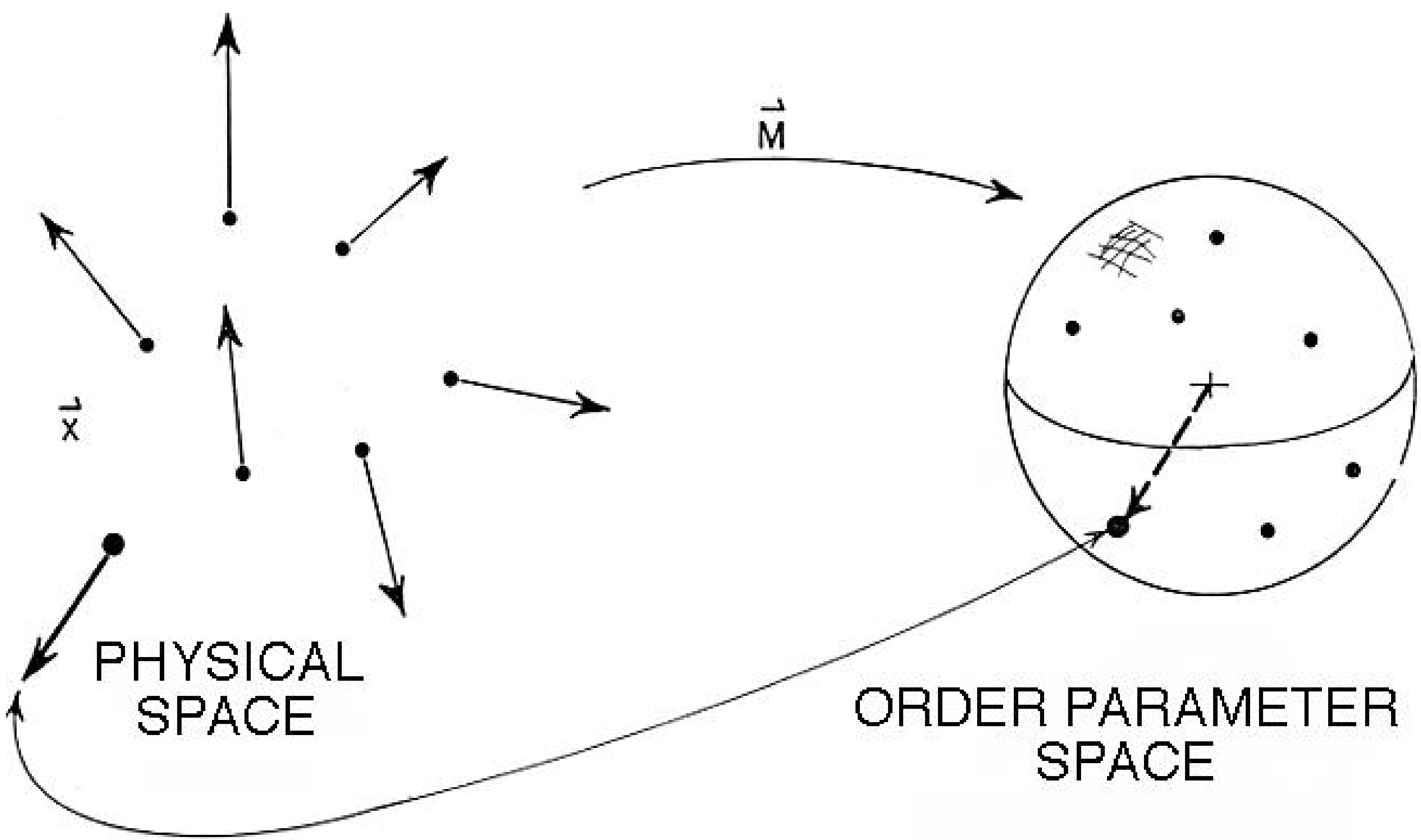




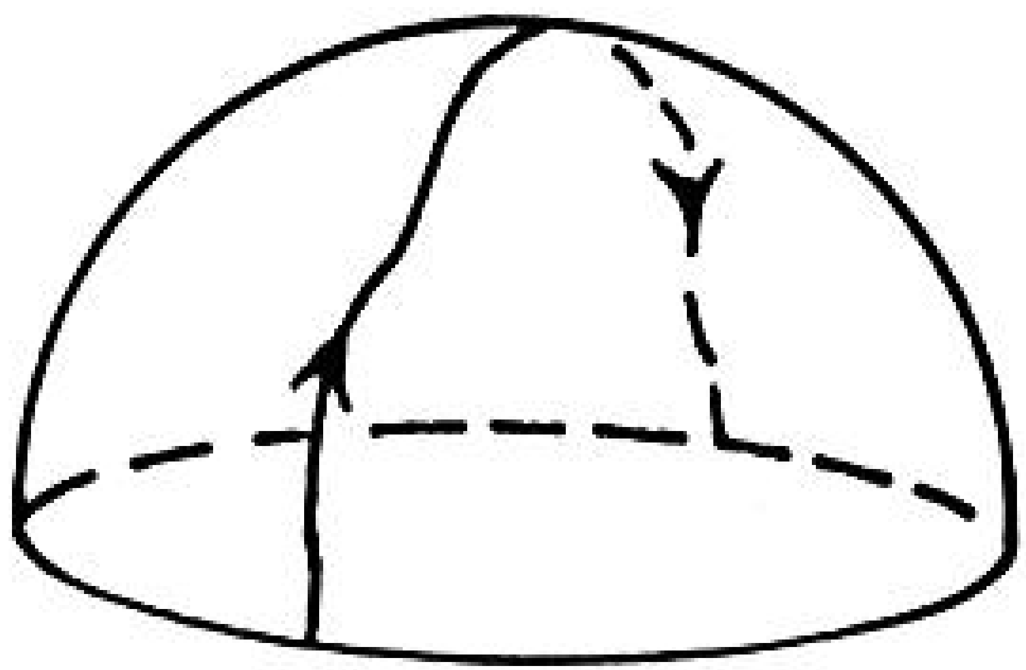
$$\vec{u} \equiv \vec{u} + a\hat{x} = \vec{u} + ma\hat{x} + na\hat{y}.$$

$$\mathcal{E} = \int dx\, (\kappa/2)(du/dx)^2.$$

Order parameters: magnets

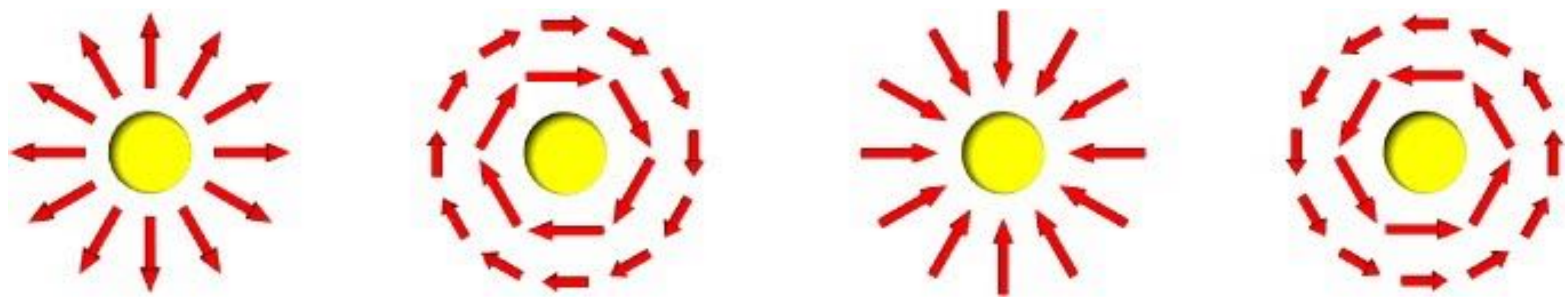


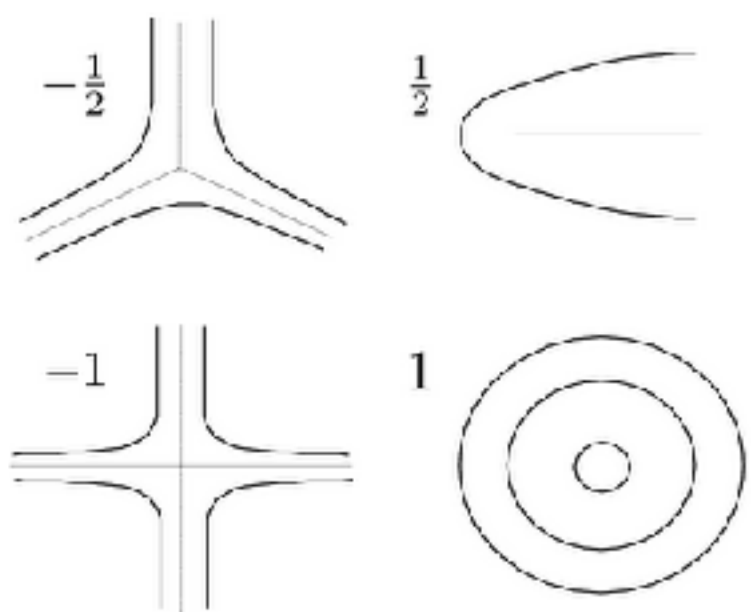
Order parameters: nematic liquid crystals

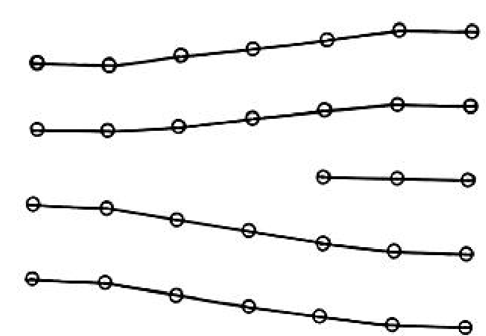


“projective plane” =
half-sphere
with opposite points on
equator identified

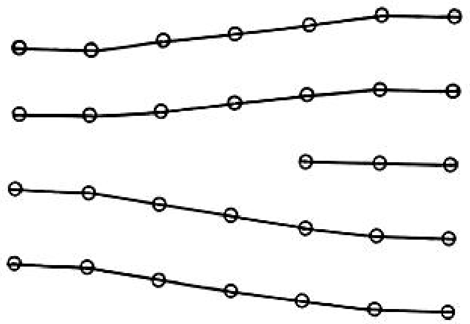
Topological defects



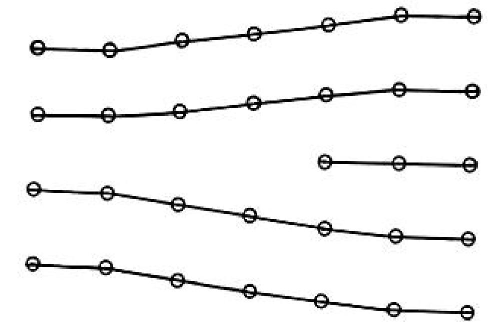


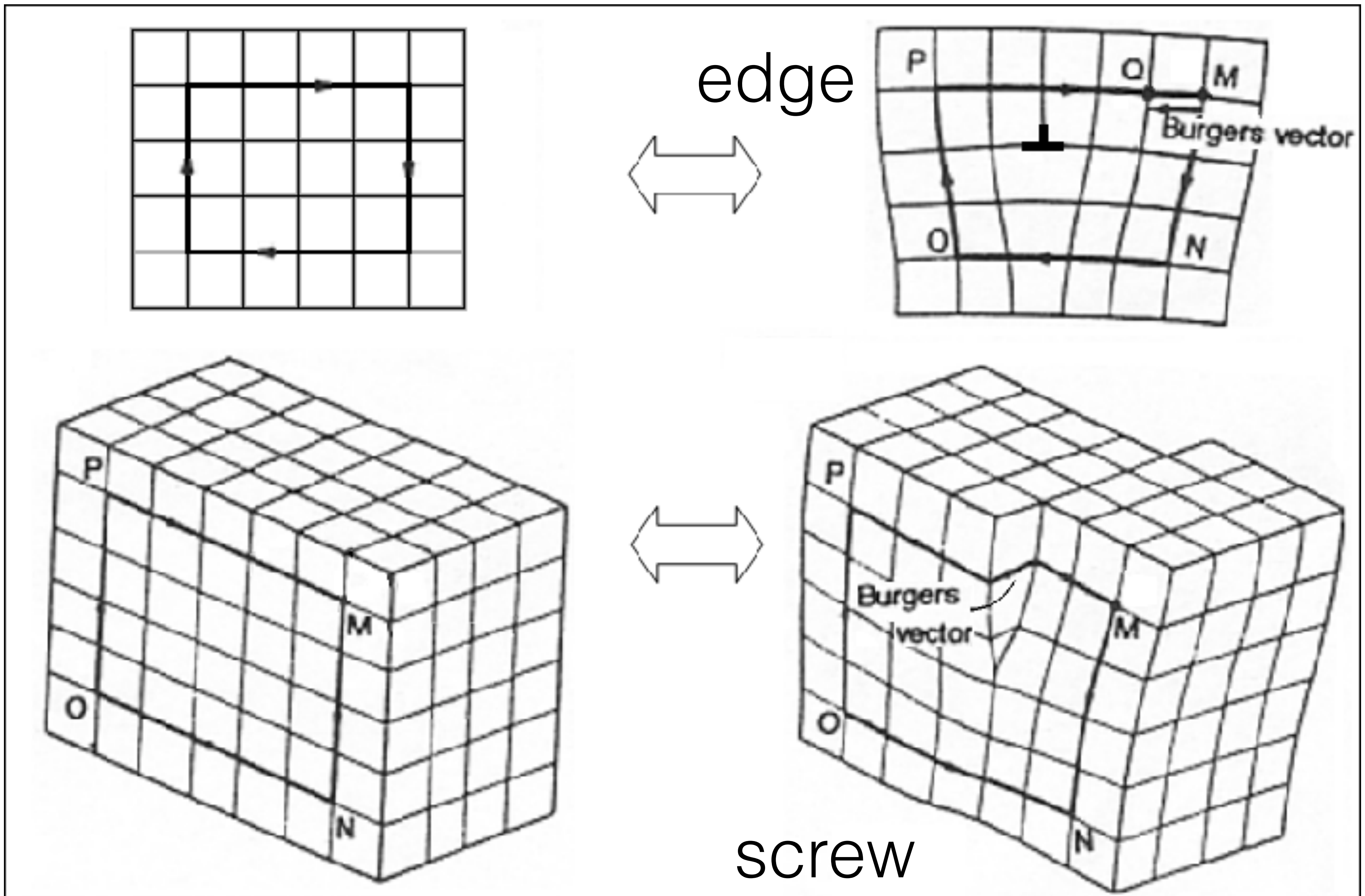


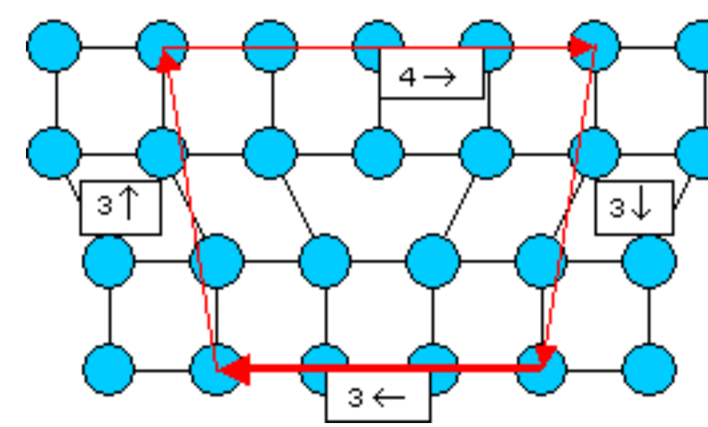
Work hardening



Dislocations

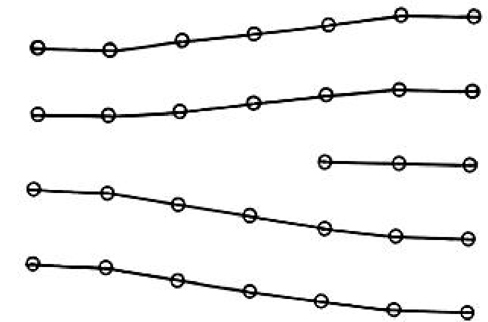


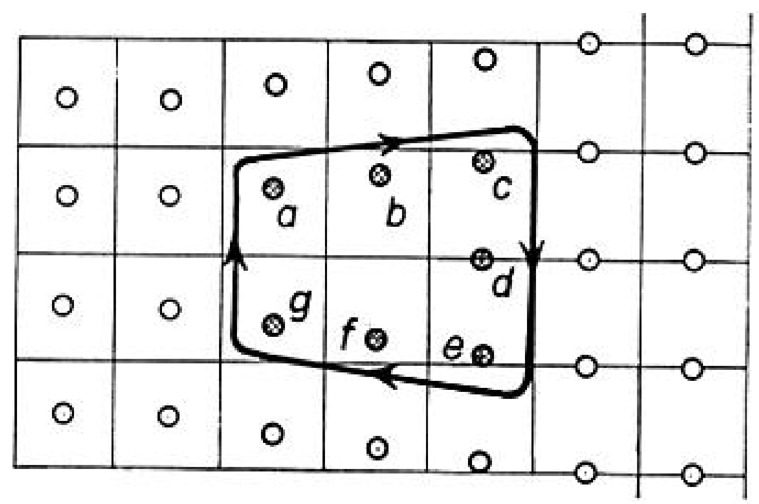


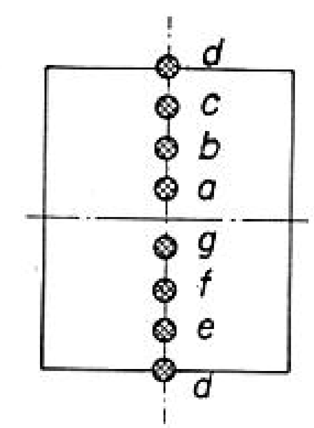


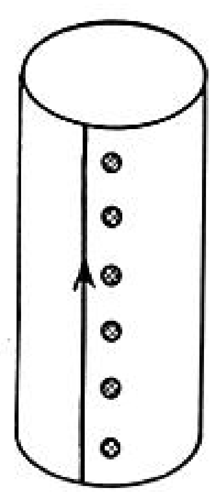
$$\|\mathbf{b}\| = (a/2)\sqrt{h^2 + k^2 + l^2}$$

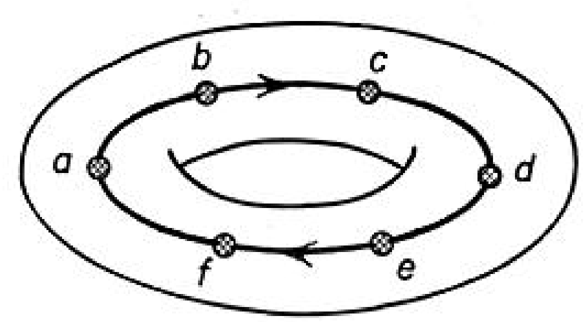
Dislocations



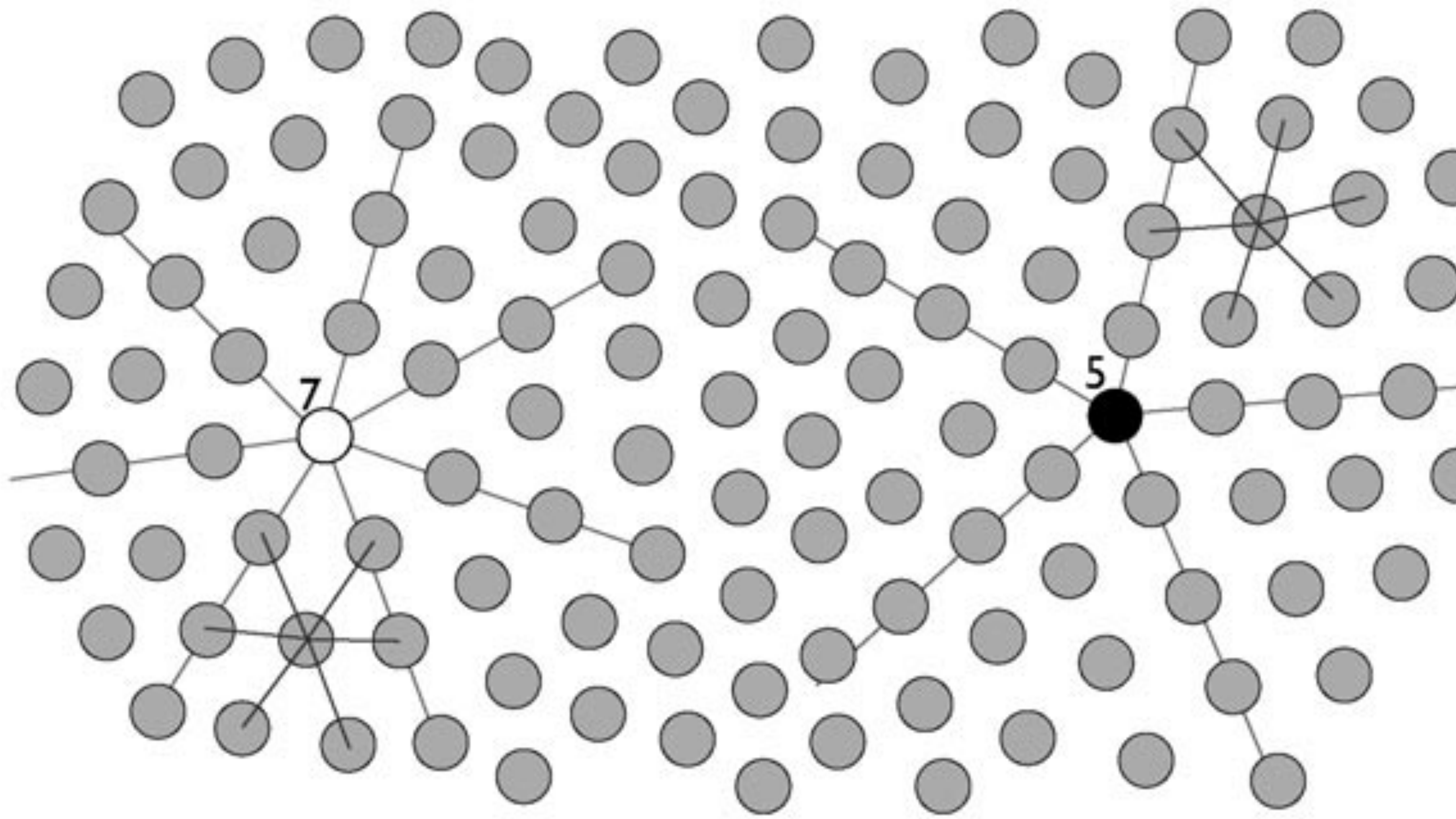






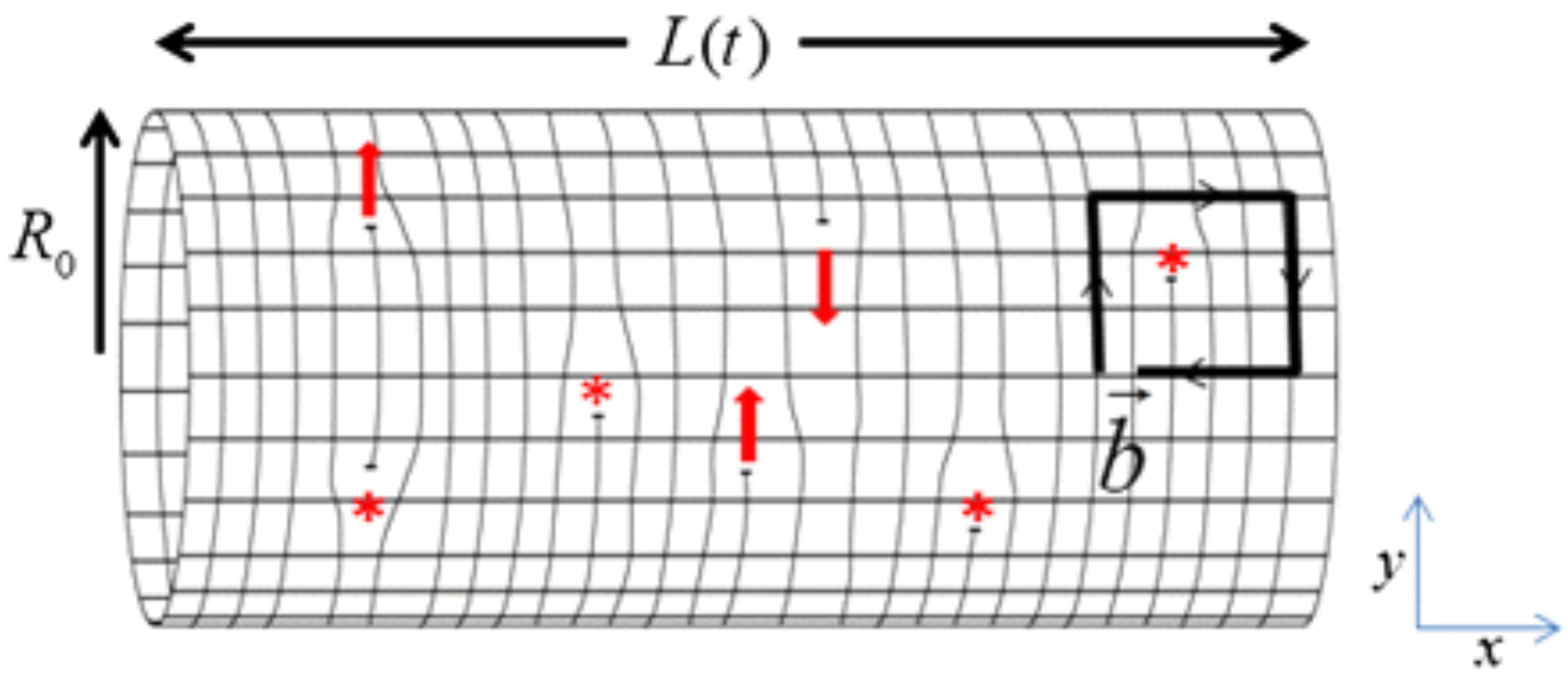


Disclination pair



Dislocation-mediated growth of bacterial cell walls

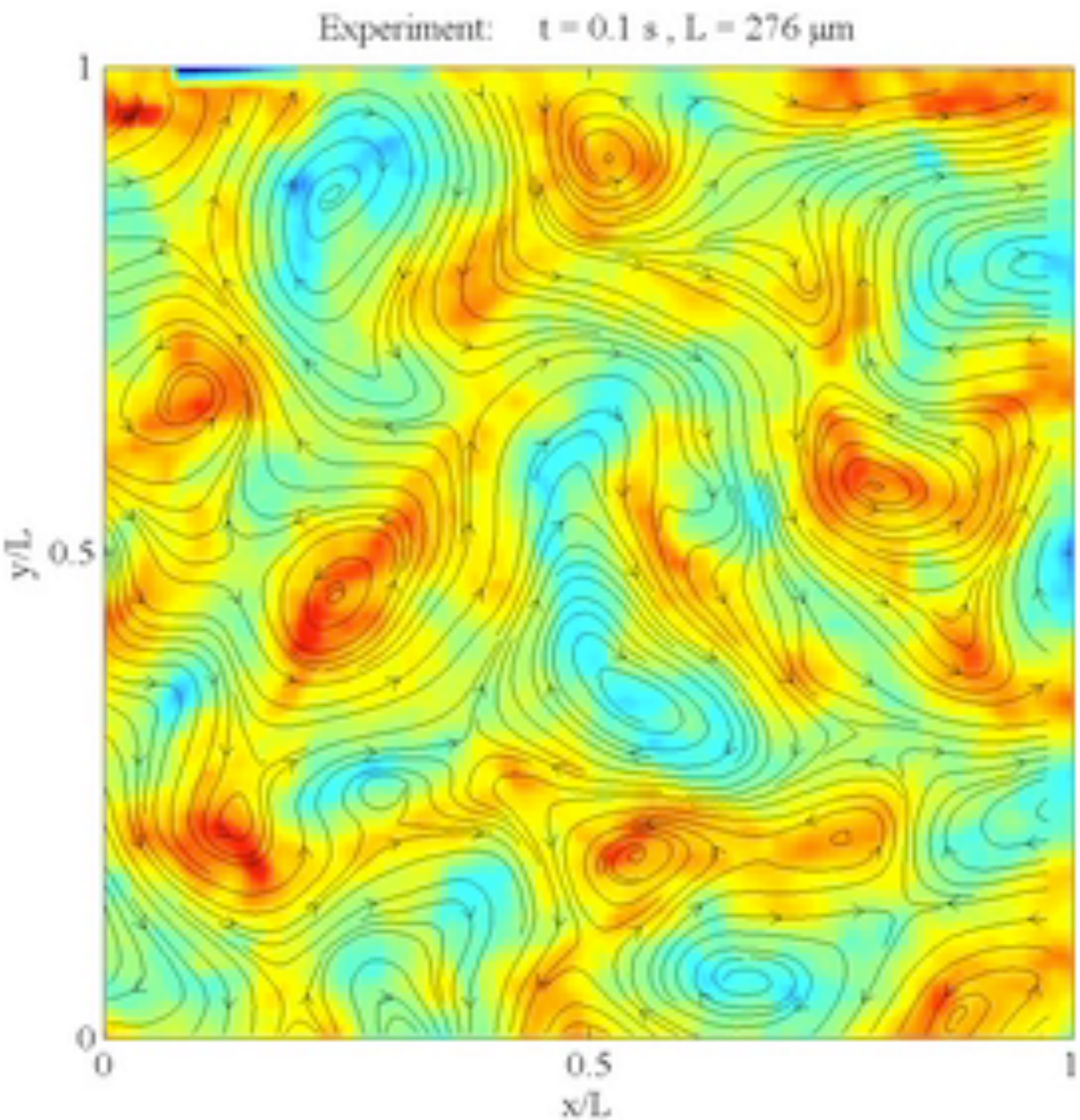
Ariel Amir and David R. Nelson[1]

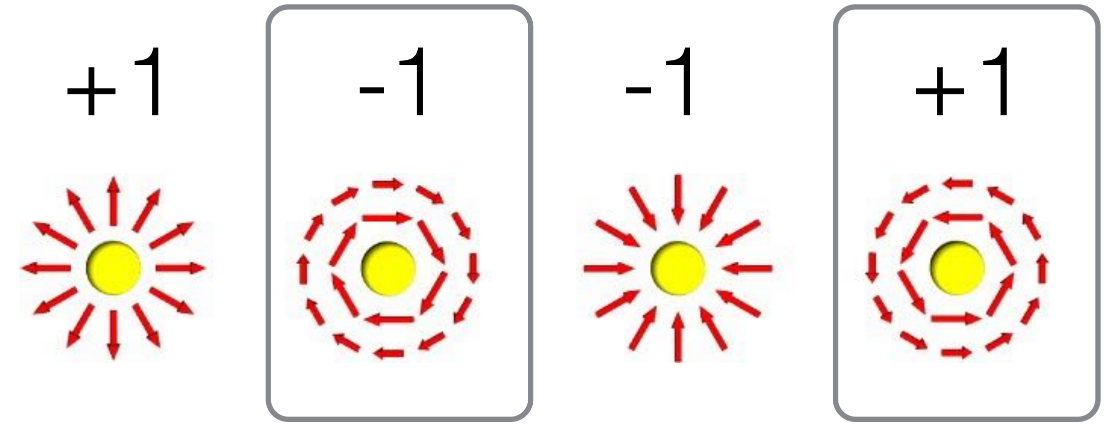


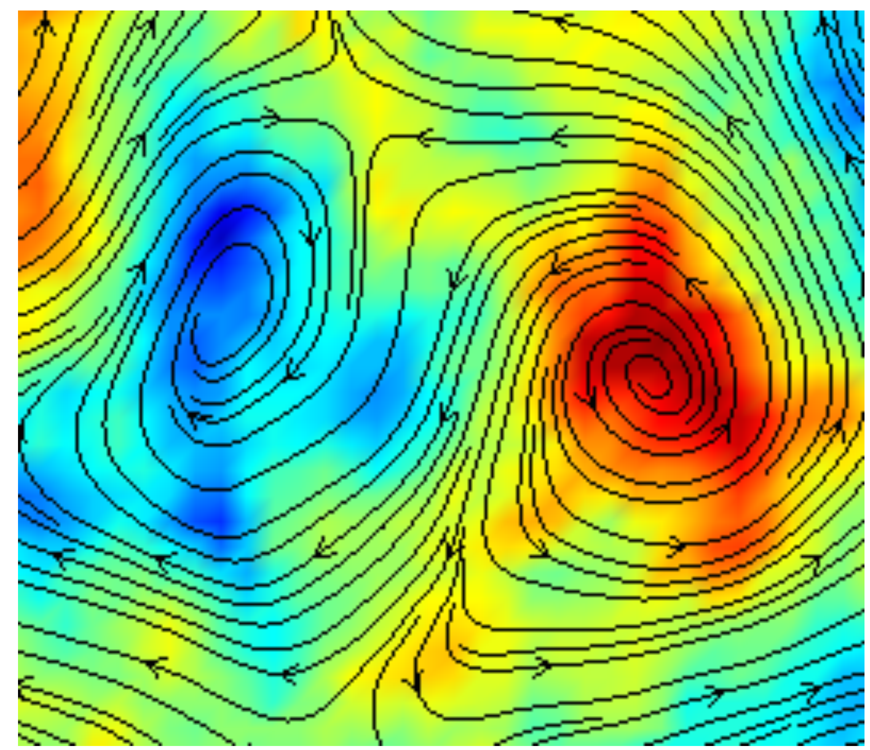
PNAS | **June 19, 2012** | vol. 109 | no. 25 | **9833–9838**

Bacterial vortices

PIV



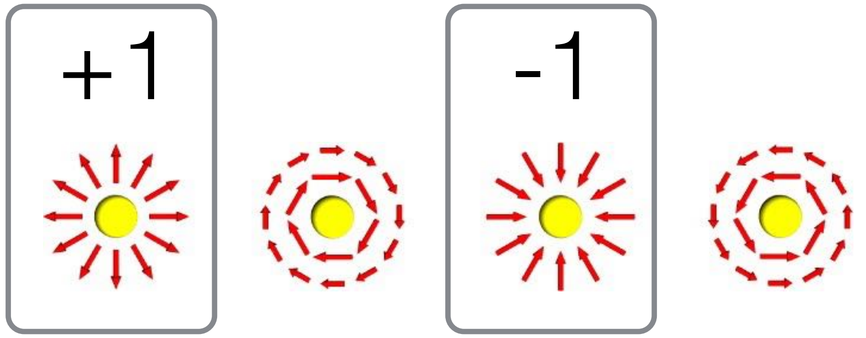




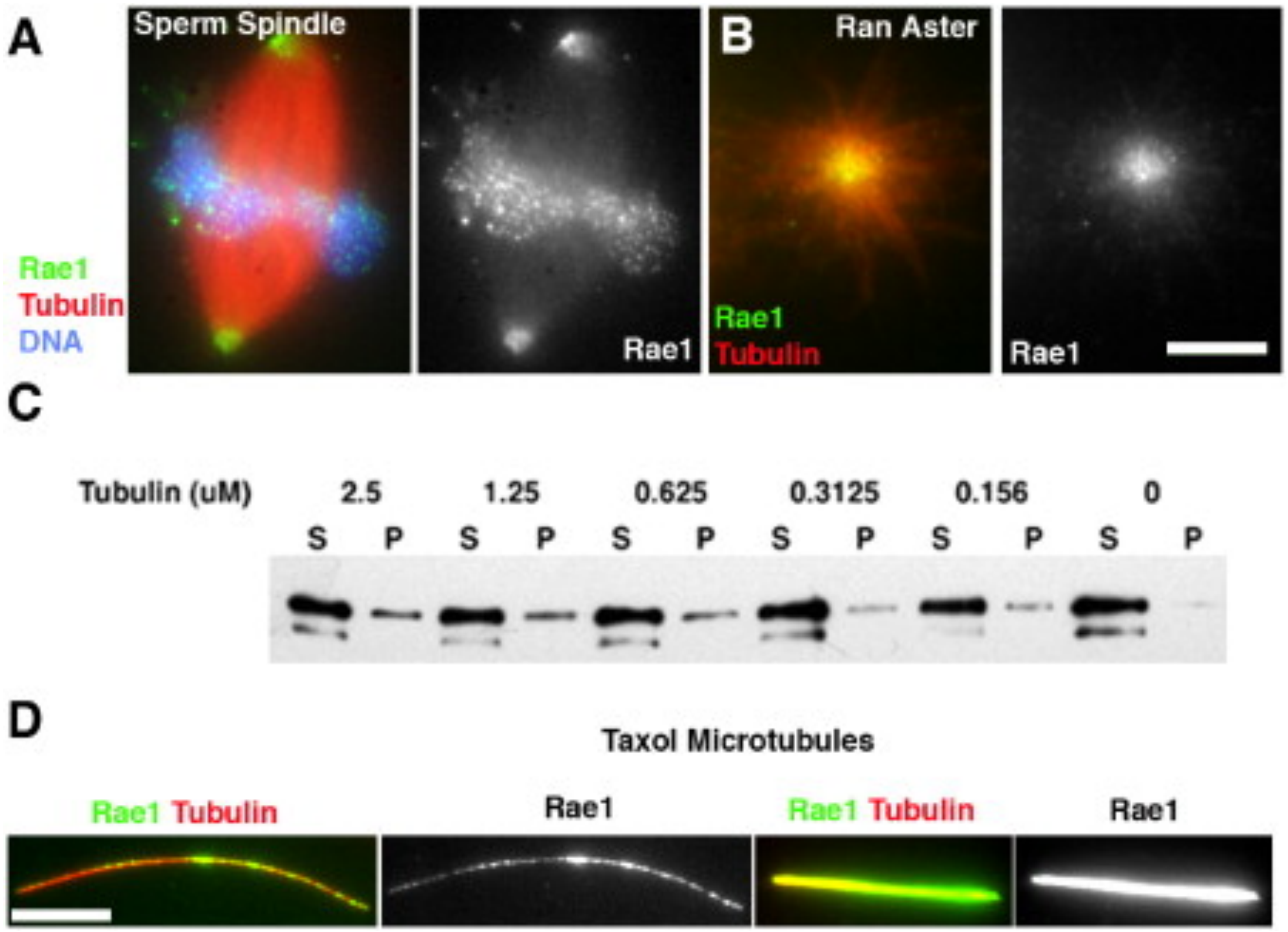
Dunkel et al PRL 2013

Microtubule asters

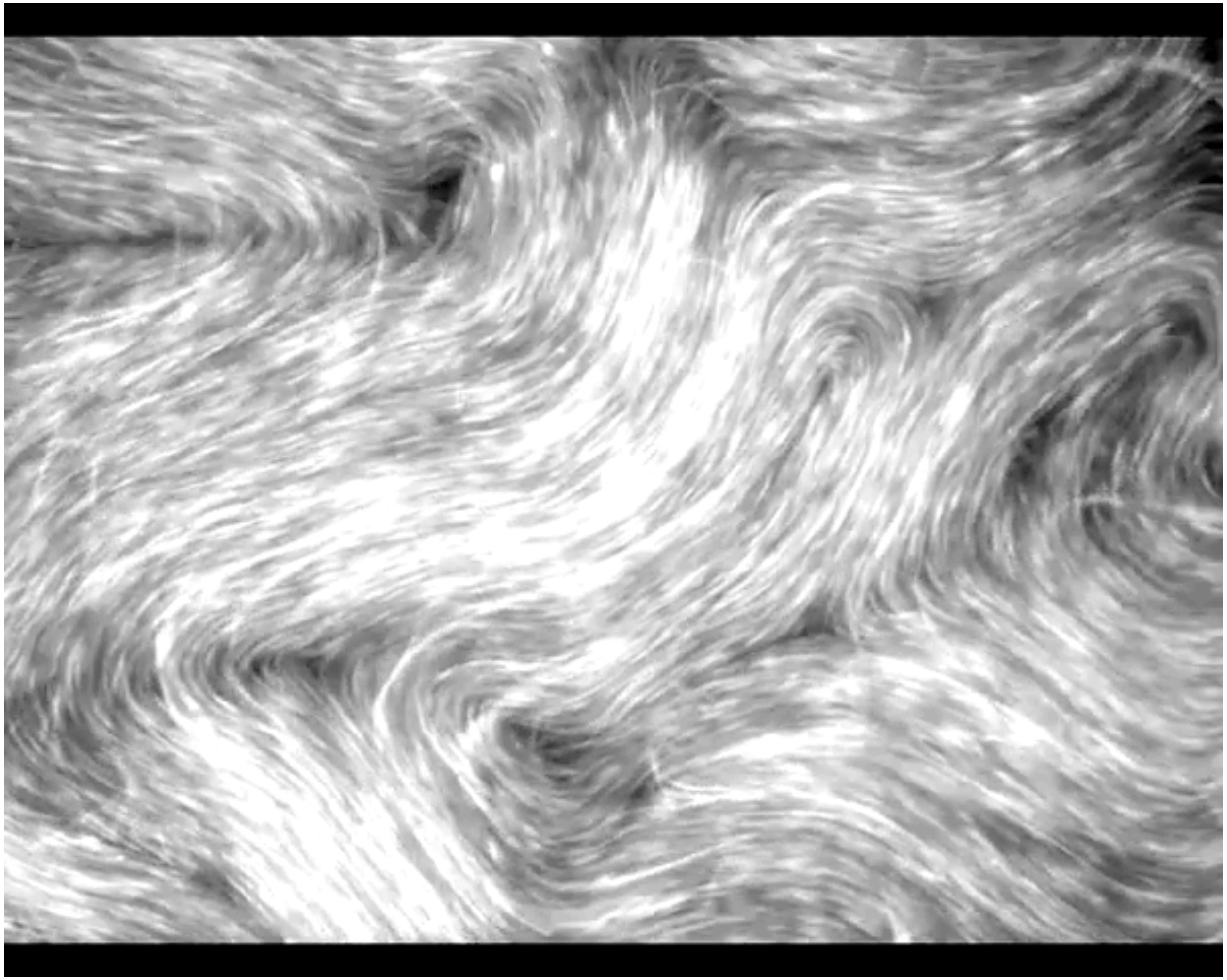
mitotic spindle organization

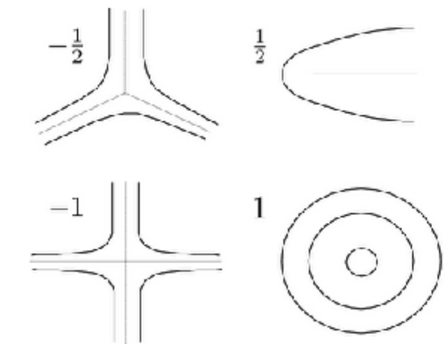


Blower et al (2005) Cell



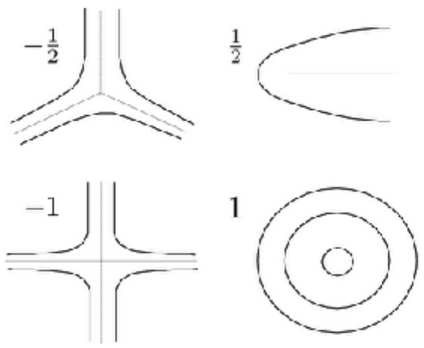
Active nematics

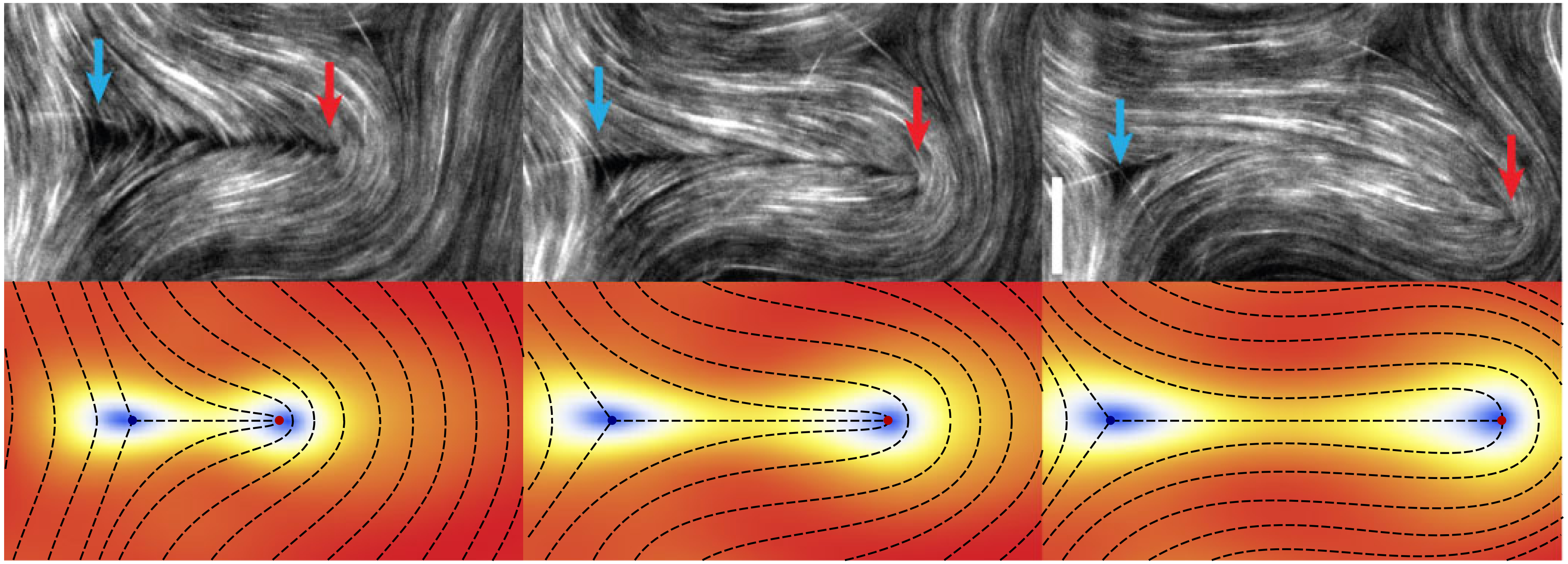




Dogic lab (Brandeis) Nature 2012

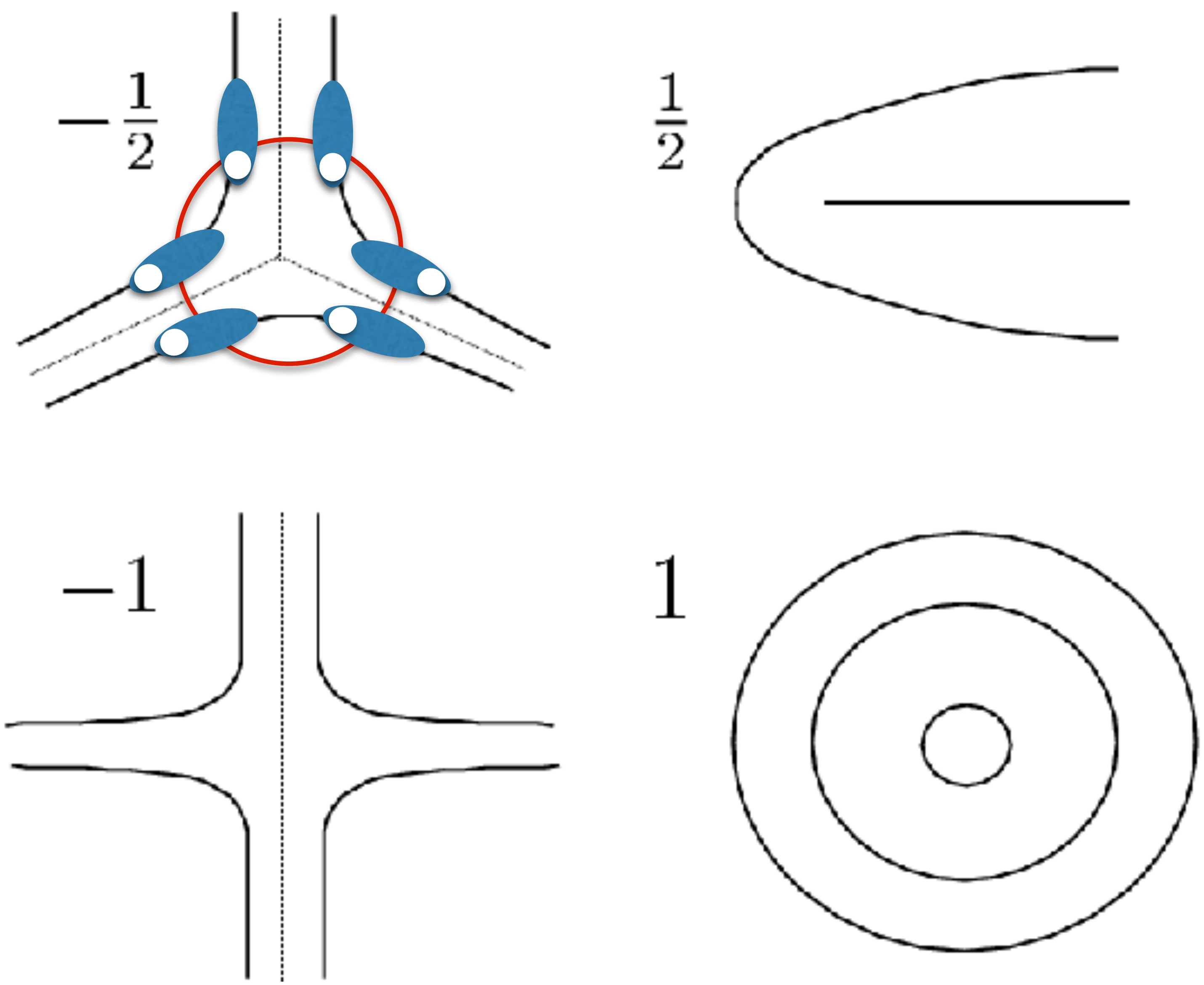
Active nematics





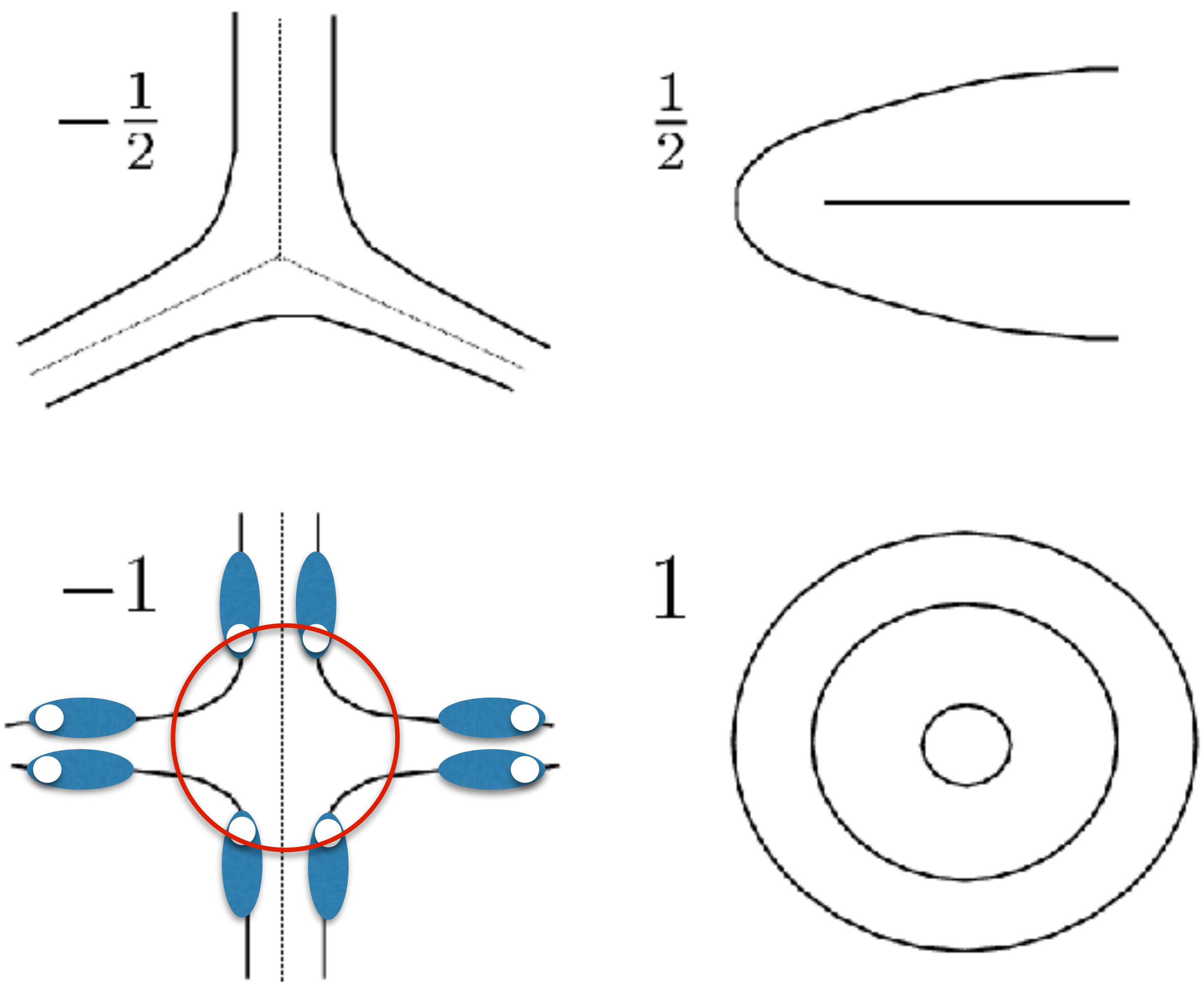
Giomi et al PRL 2012

Defects in nematics



winding number

Defects in nematics

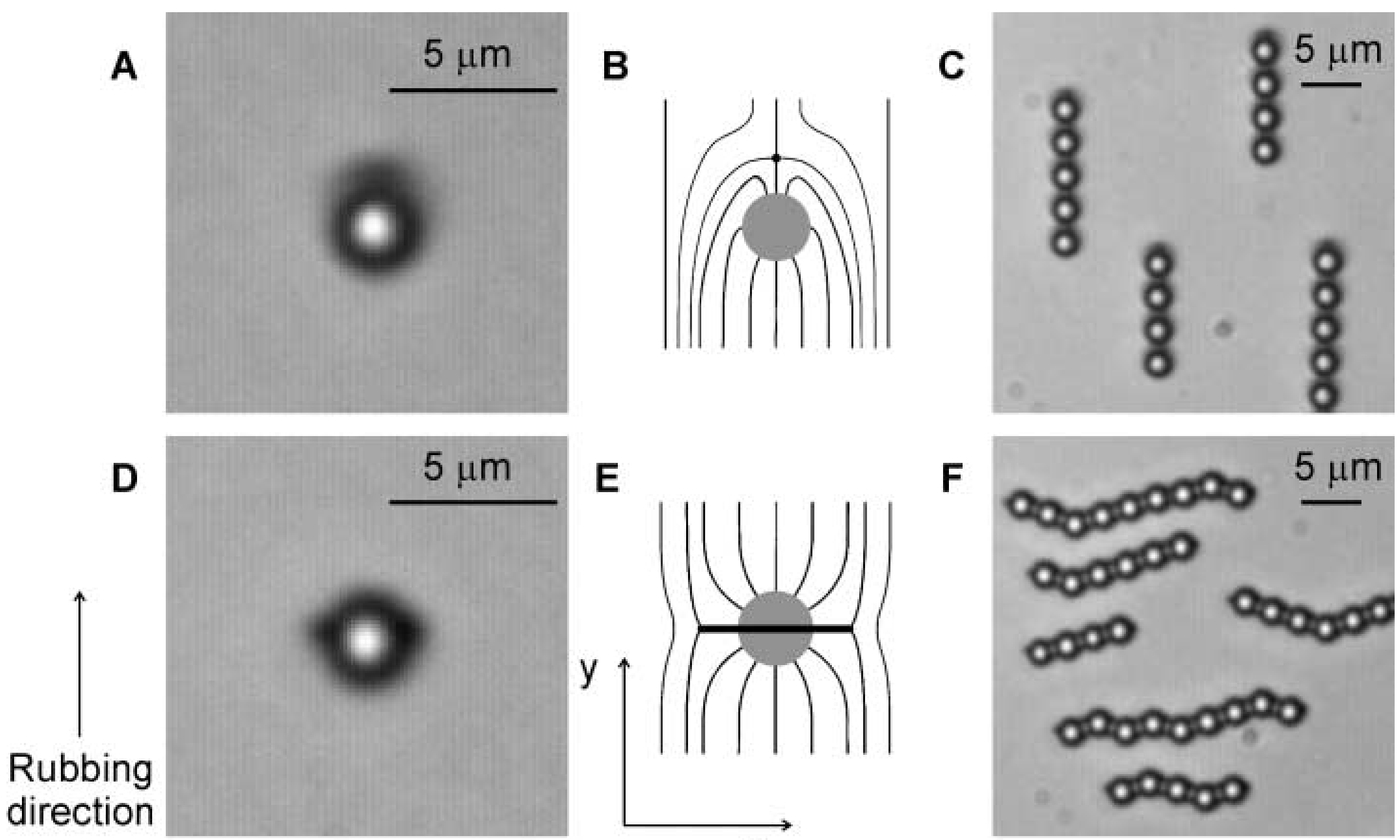


winding number

Two-Dimensional Nematic Colloidal Crystals Self-Assembled by Topological Defects

Igor Musevic *et al.*

Science **313**, 954 (2006);
DOI: 10.1126/science.1129660



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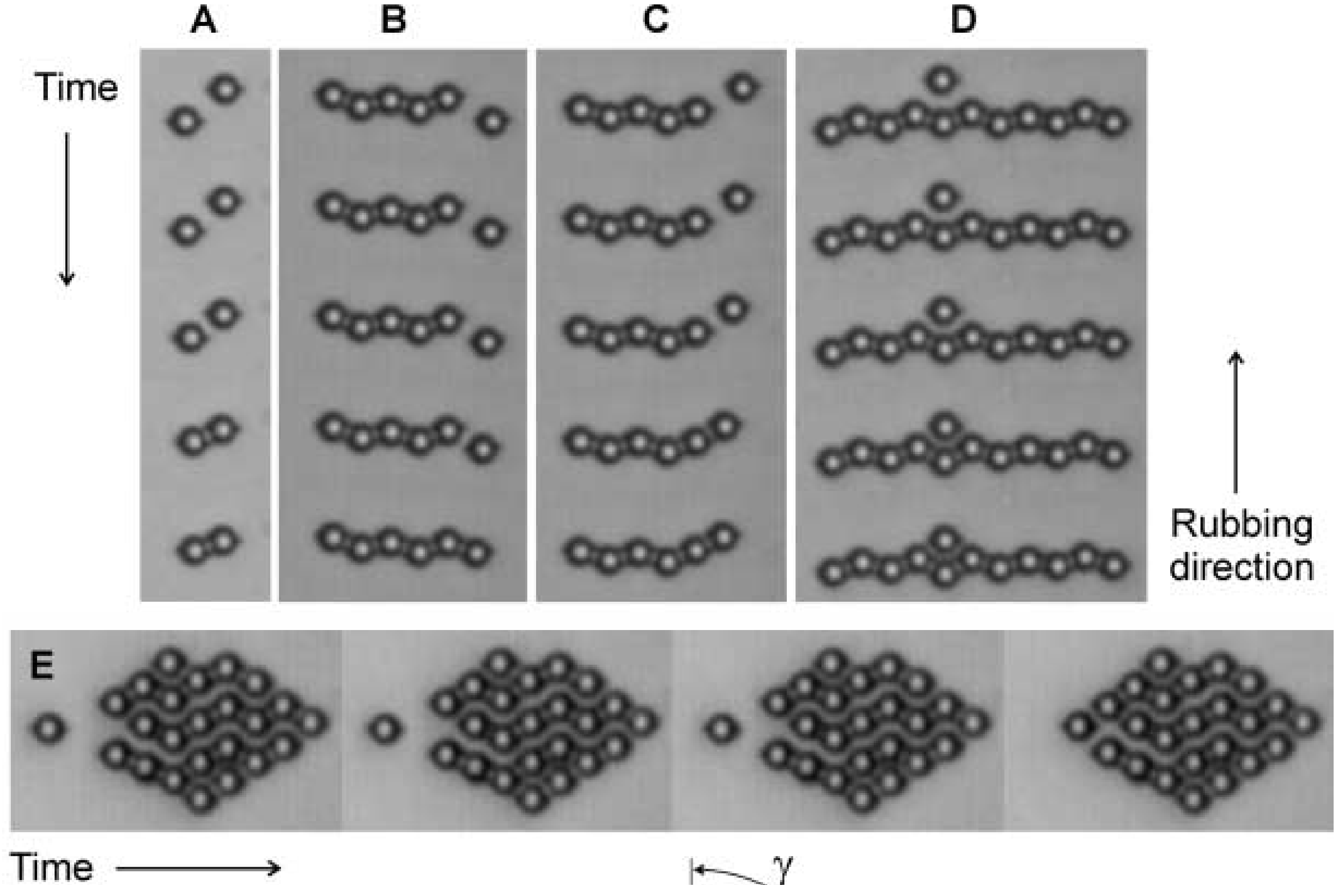
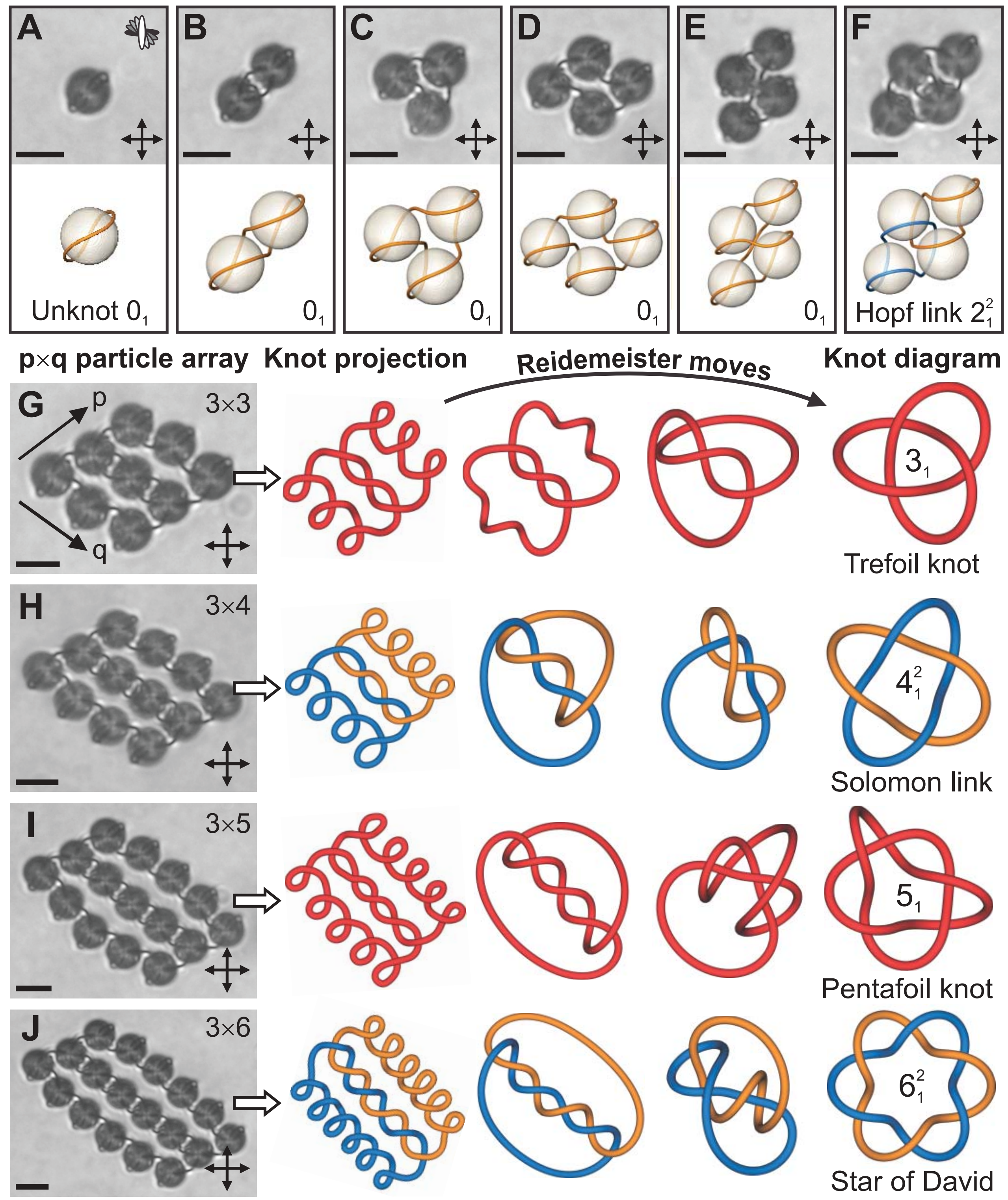


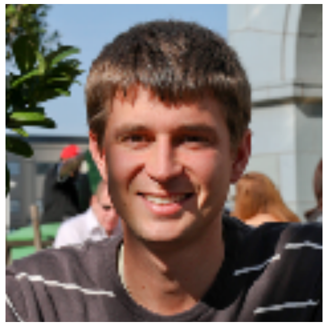
Reconfigurable Knots and Links in Chiral Nematic Colloids

Uros Tkalec *et al.*

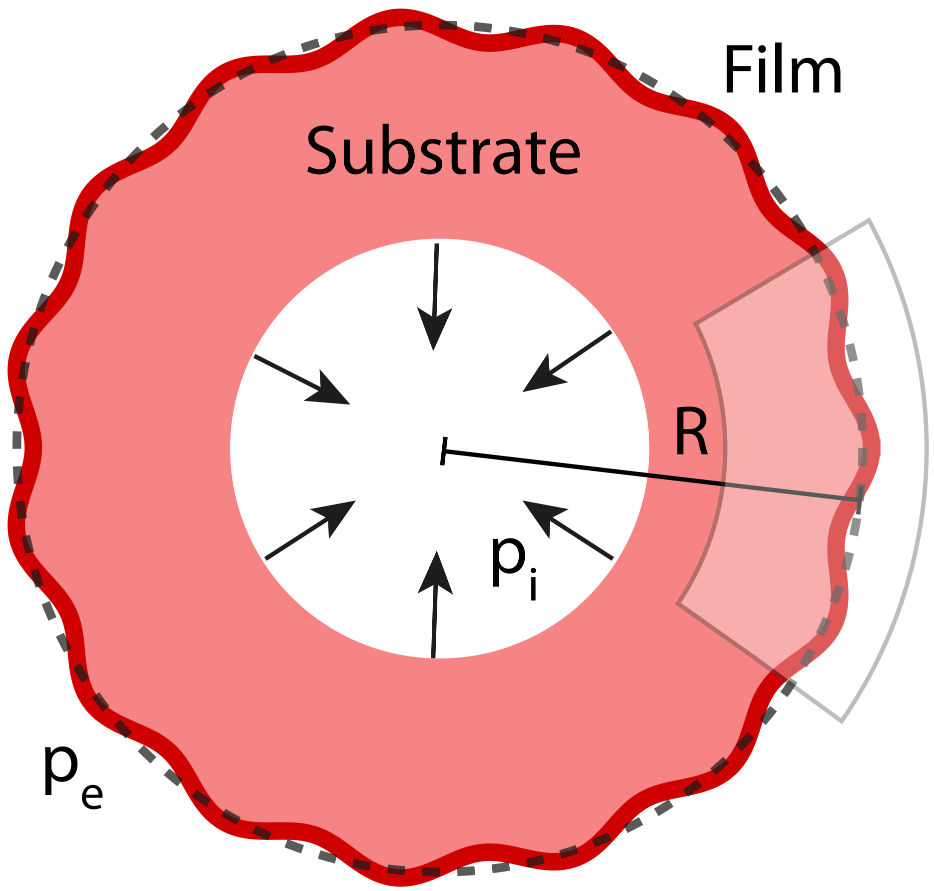
Science **333**, 62 (2011);
DOI: 10.1126/science.1205705



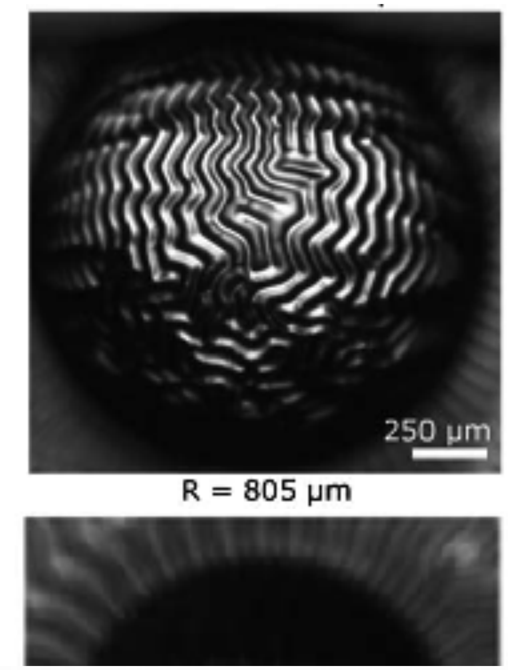
Experiment


Denis Terwagne

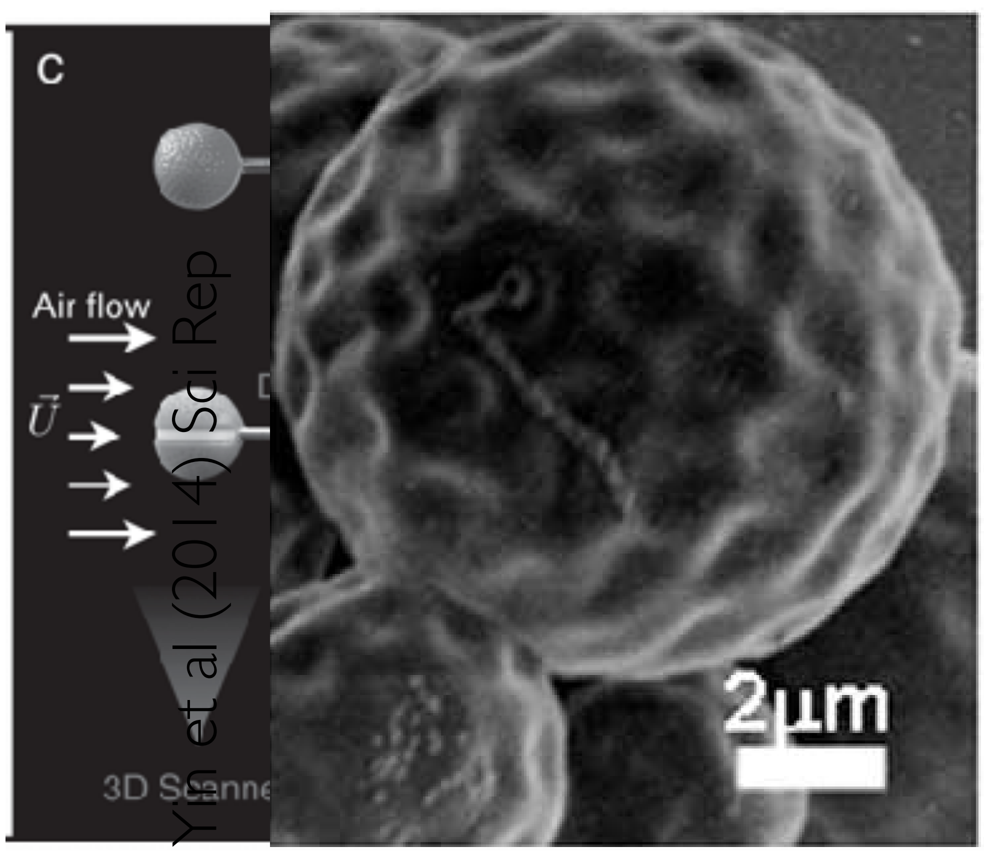

Pedro Reis



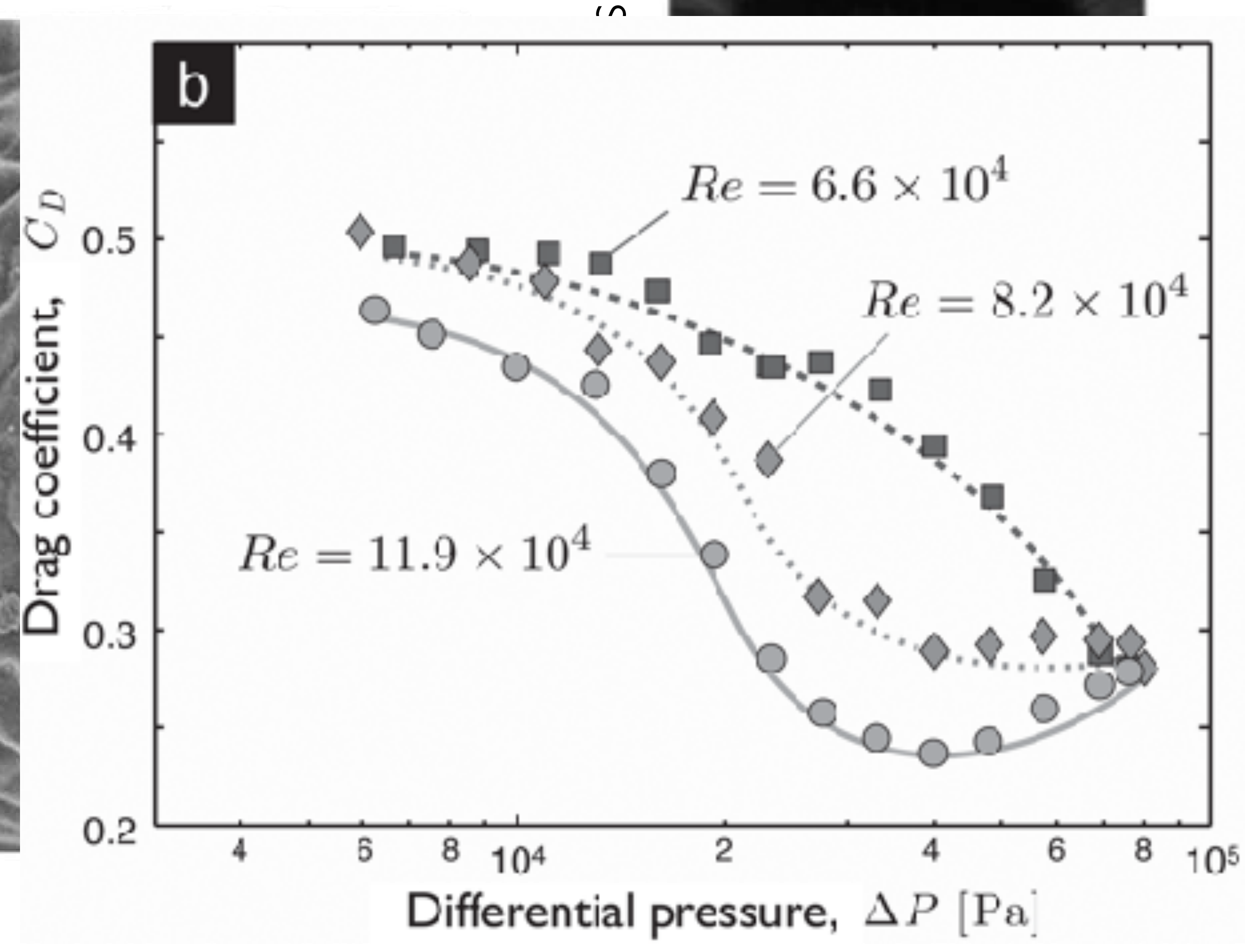
Curvature / stress-induced wrinkling transitions



sby (2013) Soft Matter



Yin et al (2014) Sci Rep



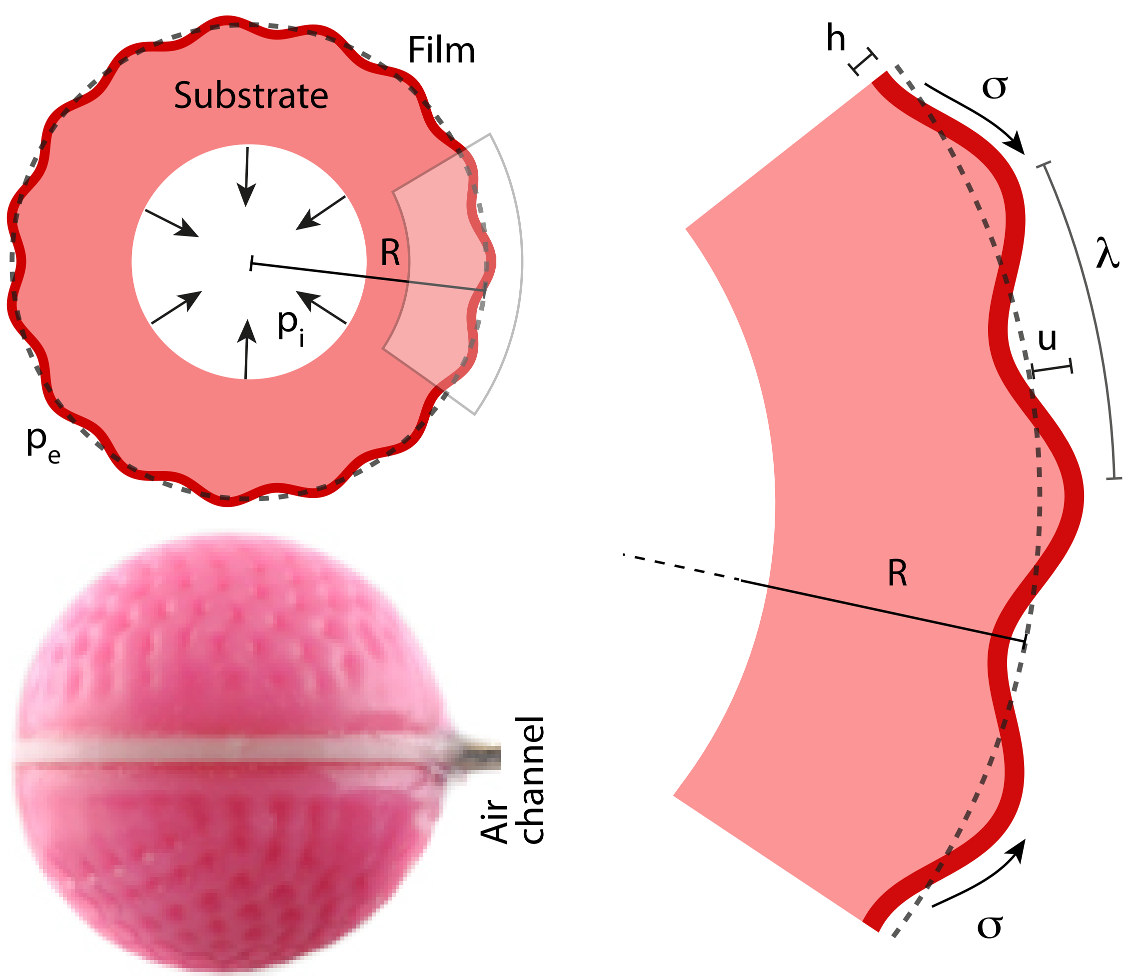
D Terwagne, M Brojan and P M Reis "Smart Morphable Surfaces for Aerodynamic Drag Control" Adv. Mater. 26 38, 6608 (2014)

5 orders of magnitude in length … similar patterns & transitions

Generalized Swift-Hohenberg theory

Norbert Stoop

$$\partial_t u = \gamma_0 \Delta u - \gamma_2 \Delta^2 u - au - bu^2 - cu^3$$
$$+ \Gamma_1 \left[(\nabla u)^2 + 2u\Delta u \right] + \Gamma_2 \left[u(\nabla u)^2 + u^2 \Delta u \right]$$



Small deformations of a **sphere**

$$(a_{\alpha\beta}) = \begin{pmatrix} (R\sin\theta_2)^2 & 0 \\ 0 & R^2 \end{pmatrix}$$

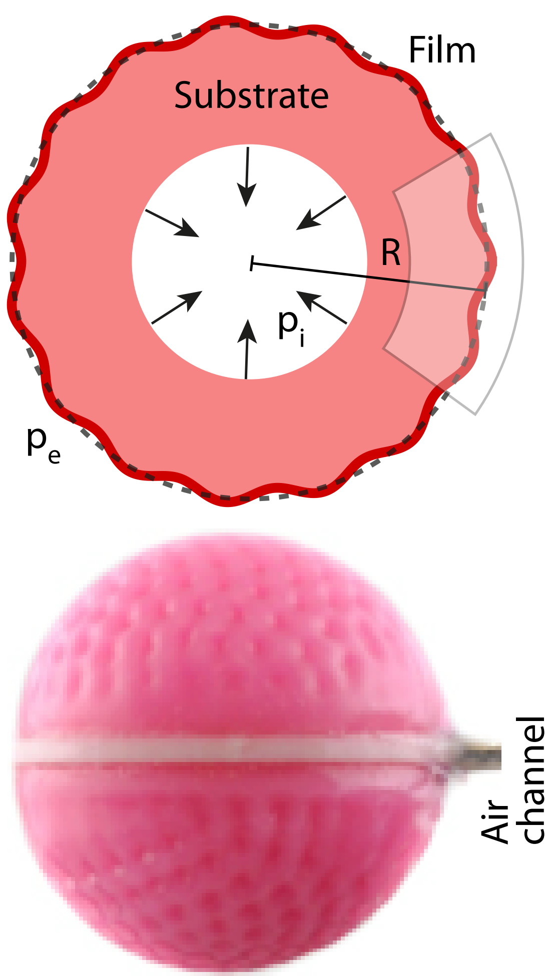
$$\triangle\psi = \nabla_\alpha \nabla^\alpha \psi = a^{\gamma\delta}\psi_{,\gamma\delta} - a^{\gamma\delta}\Gamma^{\lambda}_{\gamma\delta}\psi_{,\lambda}$$

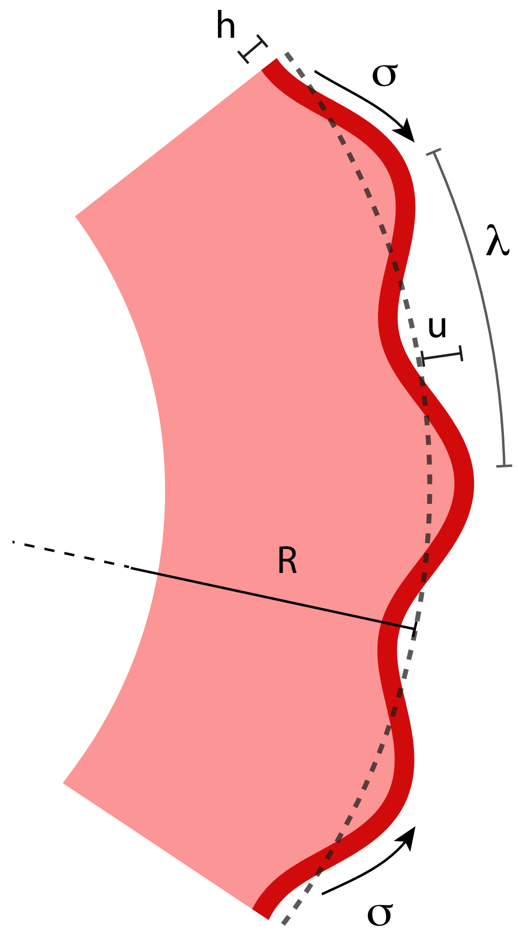
Nature Materials 2015 (joint work with Reis lab MIT MechE)

Generalized Swift-Hohenberg theory

Norbert Stoop

$$\partial_t u = \gamma_0 \Delta u - \gamma_2 \Delta^2 u - au - bu^2 - cu^3$$
$$+ \Gamma_1 \left[(\nabla u)^2 + 2u\Delta u \right] + \Gamma_2 \left[u(\nabla u)^2 + u^2 \Delta u \right]$$





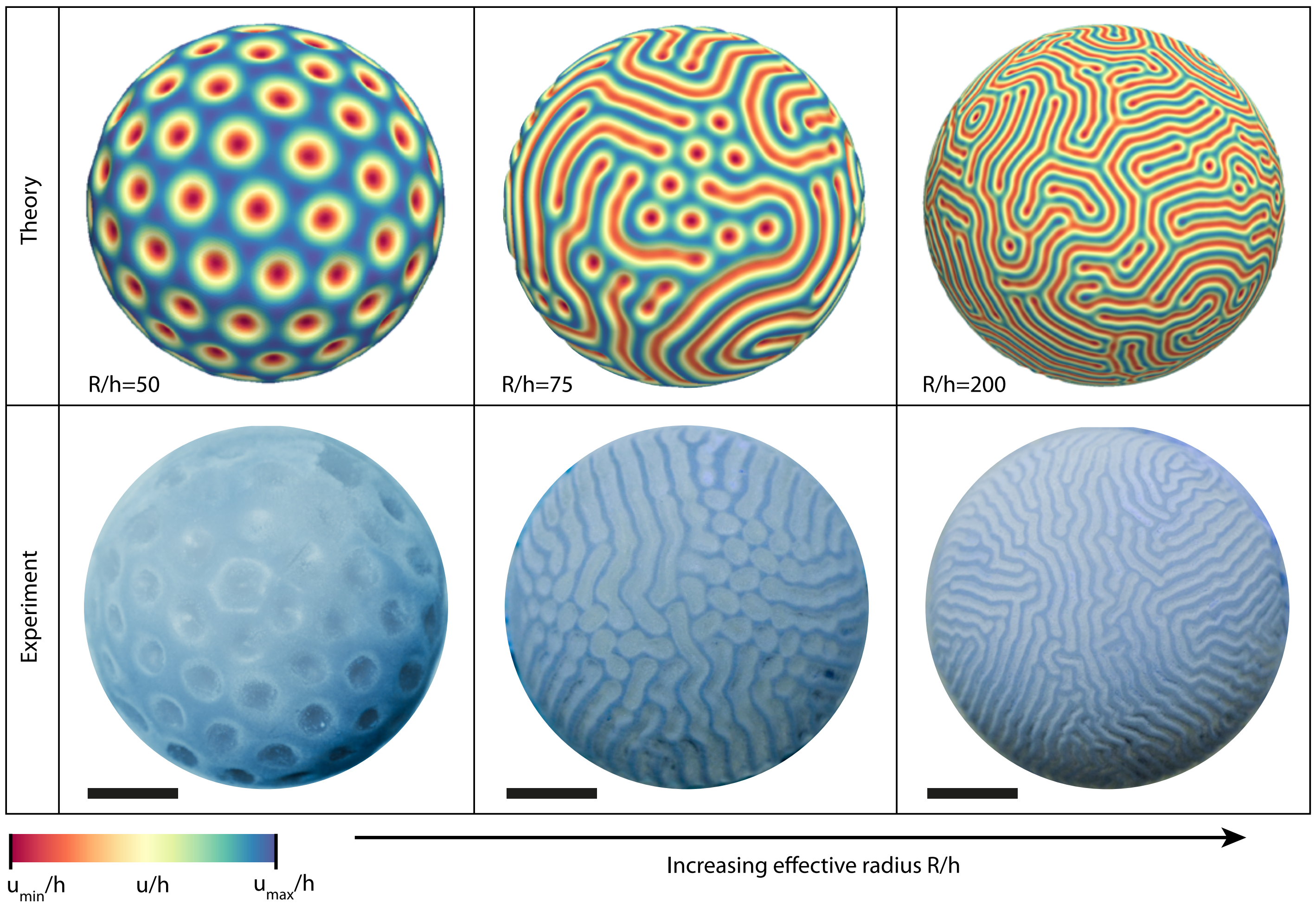
$$\gamma_0 = \frac{\kappa^2}{3} - \frac{1}{6}\sqrt{\eta^{4/3} + 24(1+\nu)\kappa^2 + 16\kappa^4}$$
$$a = \frac{\eta^{4/3}}{12} + \frac{6(1+\nu) - \eta^{2/3}}{3}\kappa^2 + \frac{\kappa^4}{3} + \tilde{a}_2 \Sigma_e$$
$$b = 3(1+\nu)\kappa^3$$
$$c = \frac{2(1+\nu)\eta^{2/3}}{3} c_1 + (1+\nu)\kappa^4$$
$$\Gamma_1 = \frac{1+\nu}{2}\kappa$$
$$\Gamma_2 = \frac{1+\nu}{2}\kappa^2$$
$$\tilde{a}_2 = -\frac{\eta^{4/3}(c + 3|\gamma_0|\Gamma_2)}{48\gamma_0^2}$$

TABLE I: List of parameters for Eq. (1) in units $h = 1$, with $\eta = 3E_s/E_f$, $\gamma_2 = 1/12$, $\Sigma_e = (\sigma/\sigma_c) - 1$ and $\kappa = h/R$. The only remaining fitting parameter of the model is c_1.

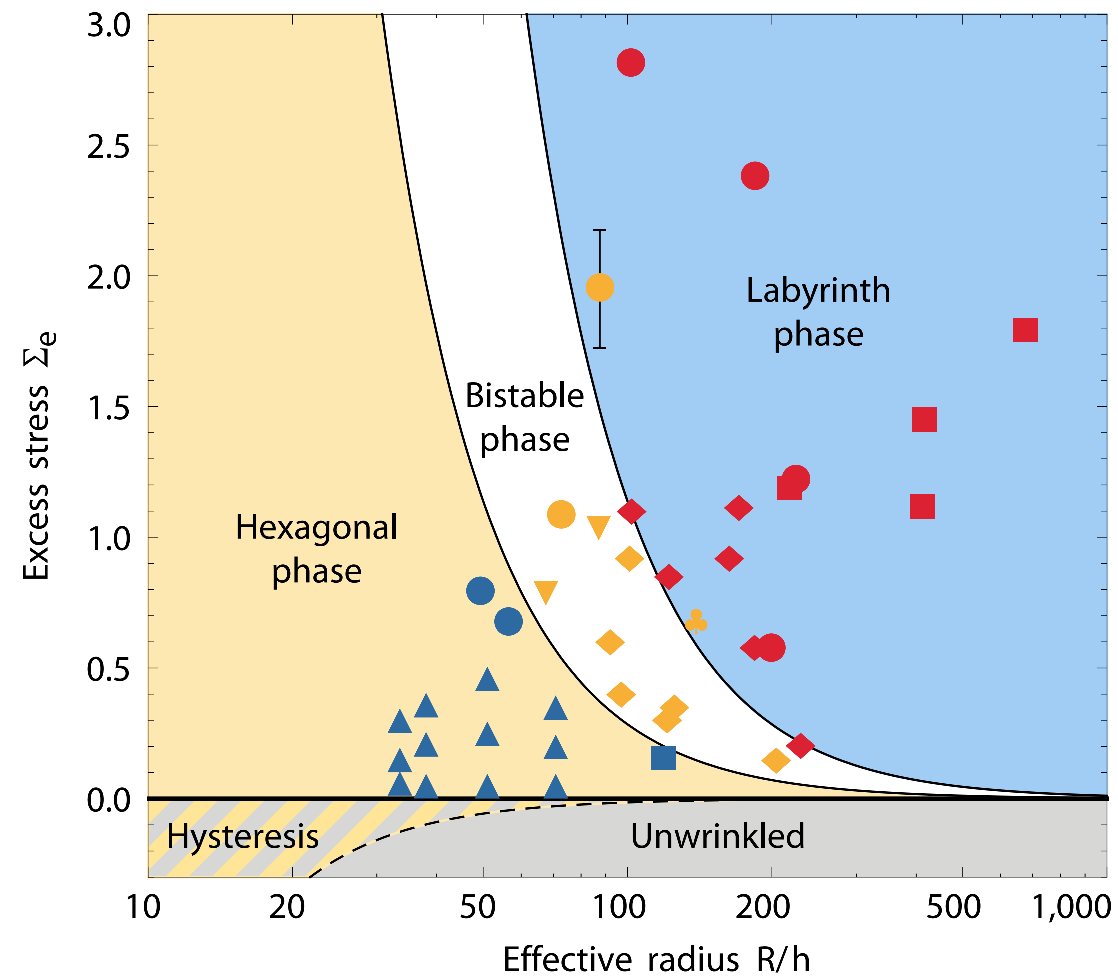
Nature Materials 2015 (joint work with Reis lab MIT MechE)

Theory correctly predicts

morphology



phase transitions

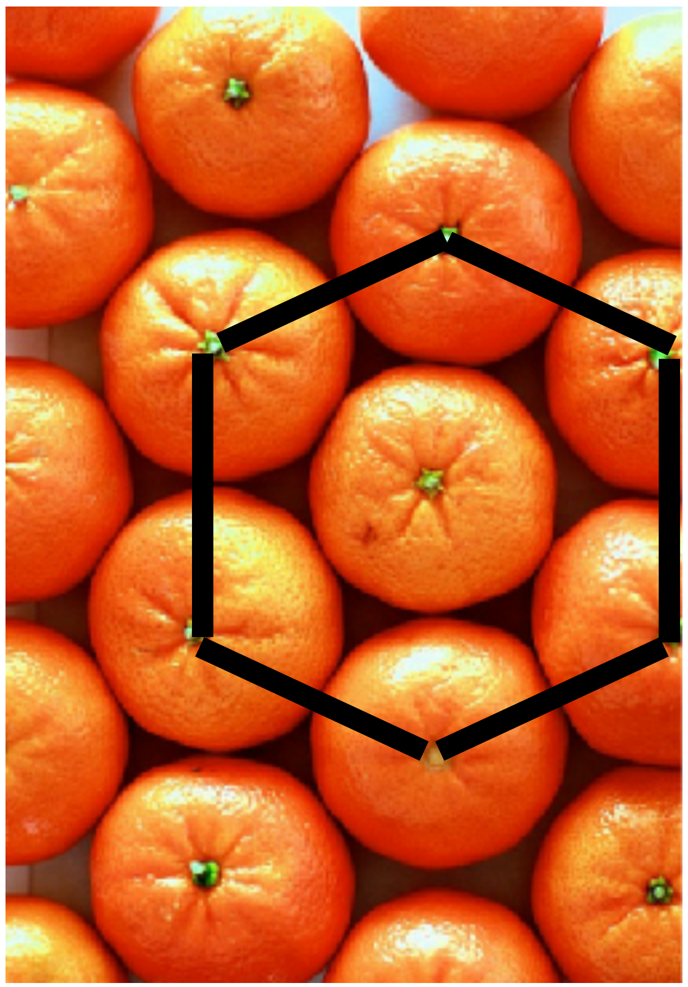


Nature Materials 2015 (joint work with Reis lab MIT MechE)

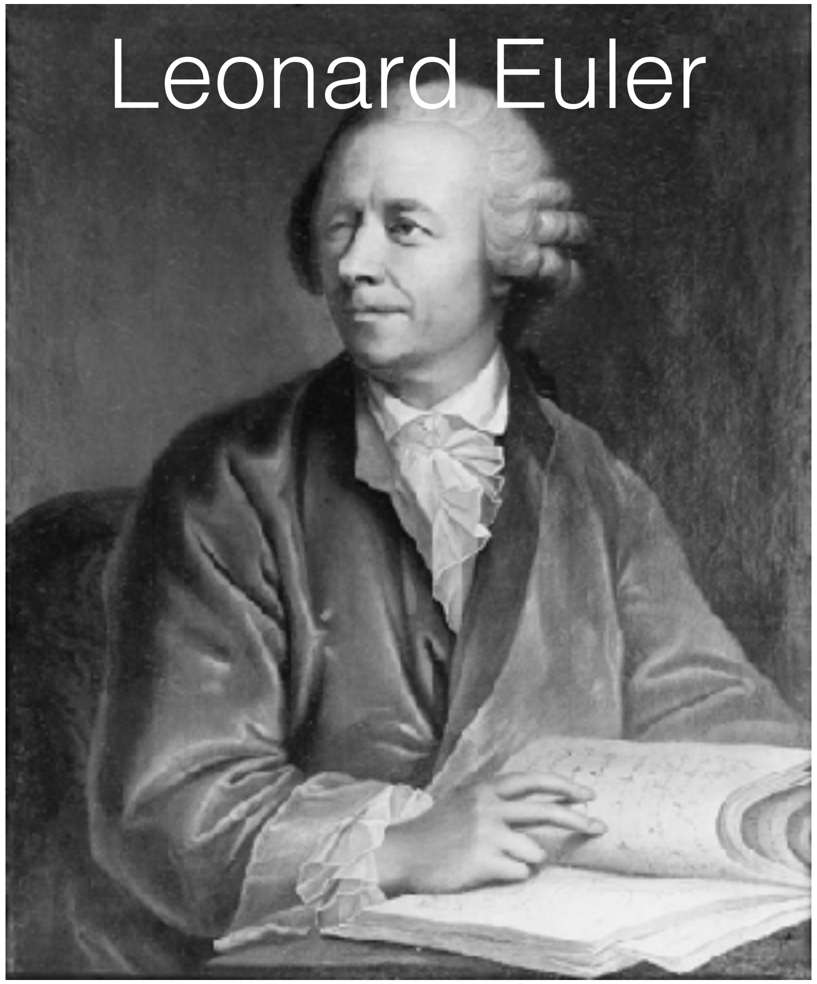
Arbitrarily curved surfaces

$$
\begin{aligned}
\mu \partial_t u = \ & \gamma_0 \triangle u - \gamma_2 \triangle^2 u - au - bu^2 - cu^3 + \\
& \frac{h}{2} \left\{ (\nu - 1) \left[b^{\alpha\beta} \nabla_\alpha u \nabla_\beta u + 2u \nabla_\beta \left(b^{\alpha\beta} \nabla_\alpha u \right) \right] + \right. \\
& \left. 2\nu \left[\mathcal{H} (\nabla u)^2 - 2 \nabla \cdot (\mathcal{H} u \nabla u) \right] \right\} + \\
& \frac{h}{2} \left[(1 - \nu) u \nabla_\beta \left(u c^{\alpha\beta} \nabla_\alpha u \right) - \nu \mathcal{R} u (\nabla u)^2 + \right. \\
& \left. \nu \nabla \cdot (\mathcal{R} u^2 \nabla u) \right]
\end{aligned}
$$

Topological defects



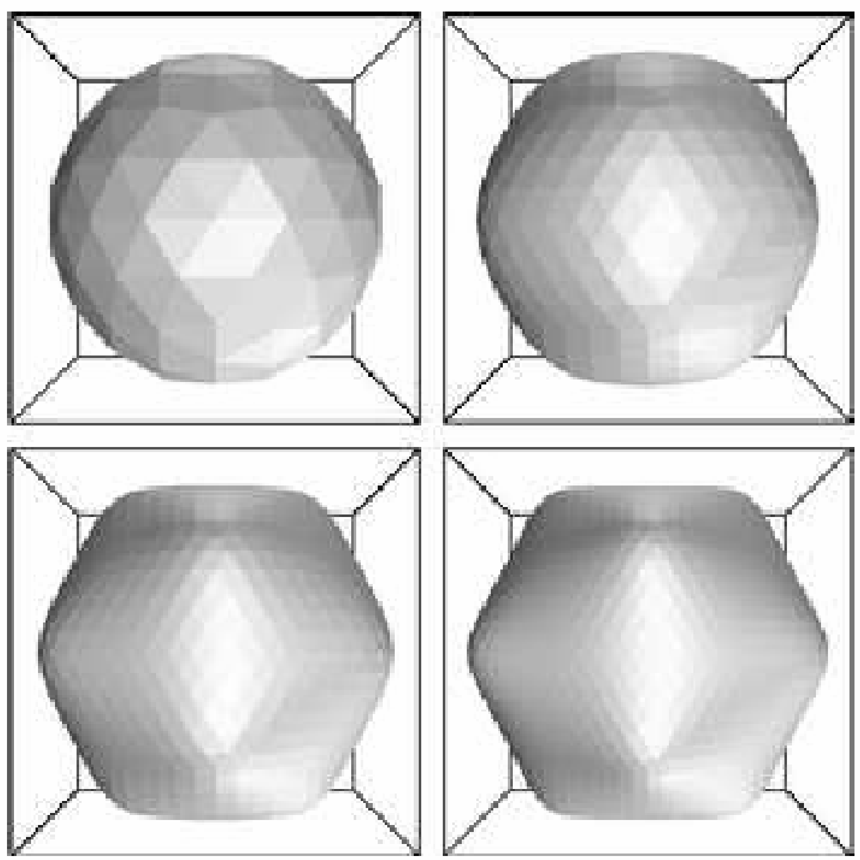
20 hexagons
12 pentagons



$$V - E + F = 2$$

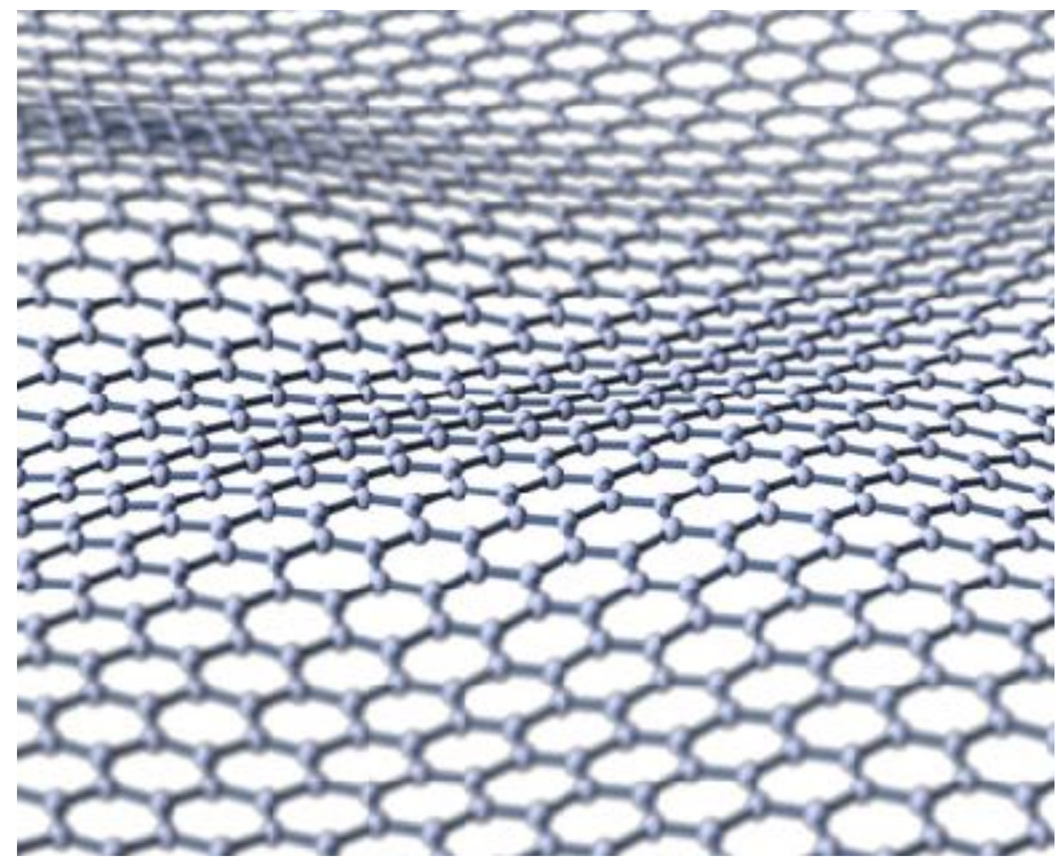
Why interesting ?

topological defects
nucleate size-induced shape transition
in viral capsids



J Lidmar, L Mirny and DR Nelson (2003) PRE

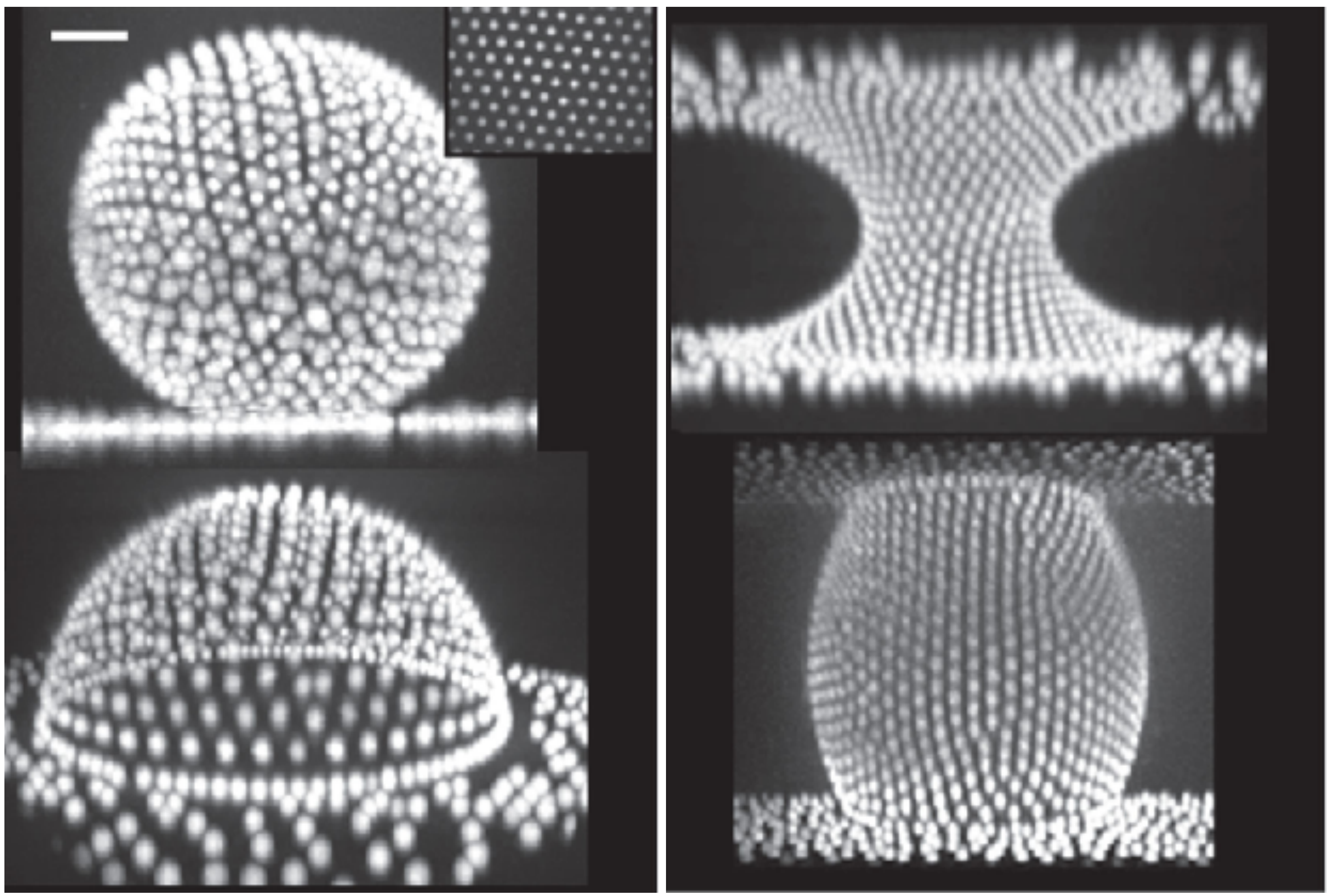
bending of graphene
introduces defects and
changes electronic properties



A Cortijo and MAH Vozmediano (2007) EPL

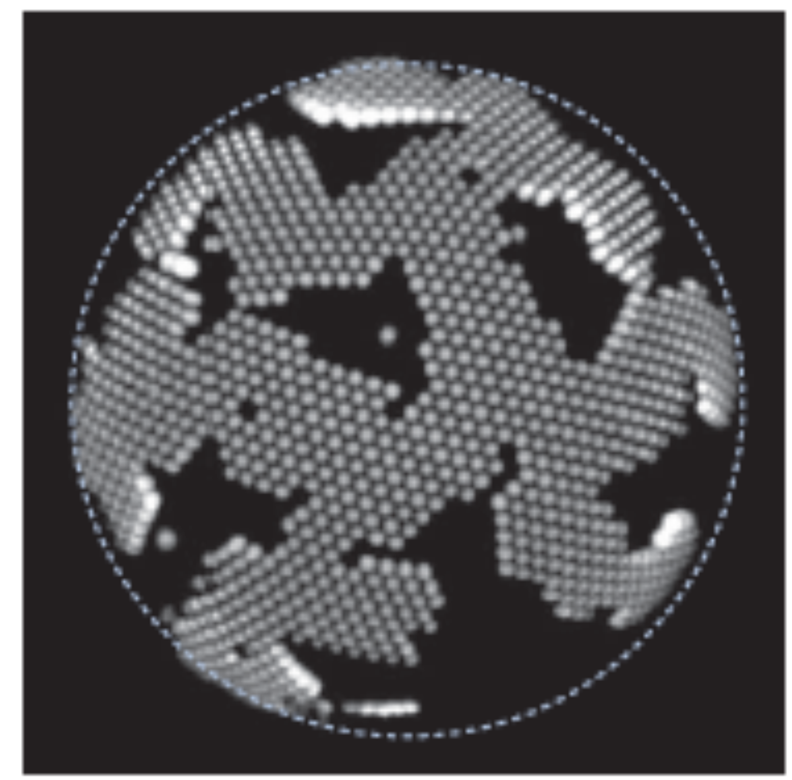
Surface crystallography

Statics



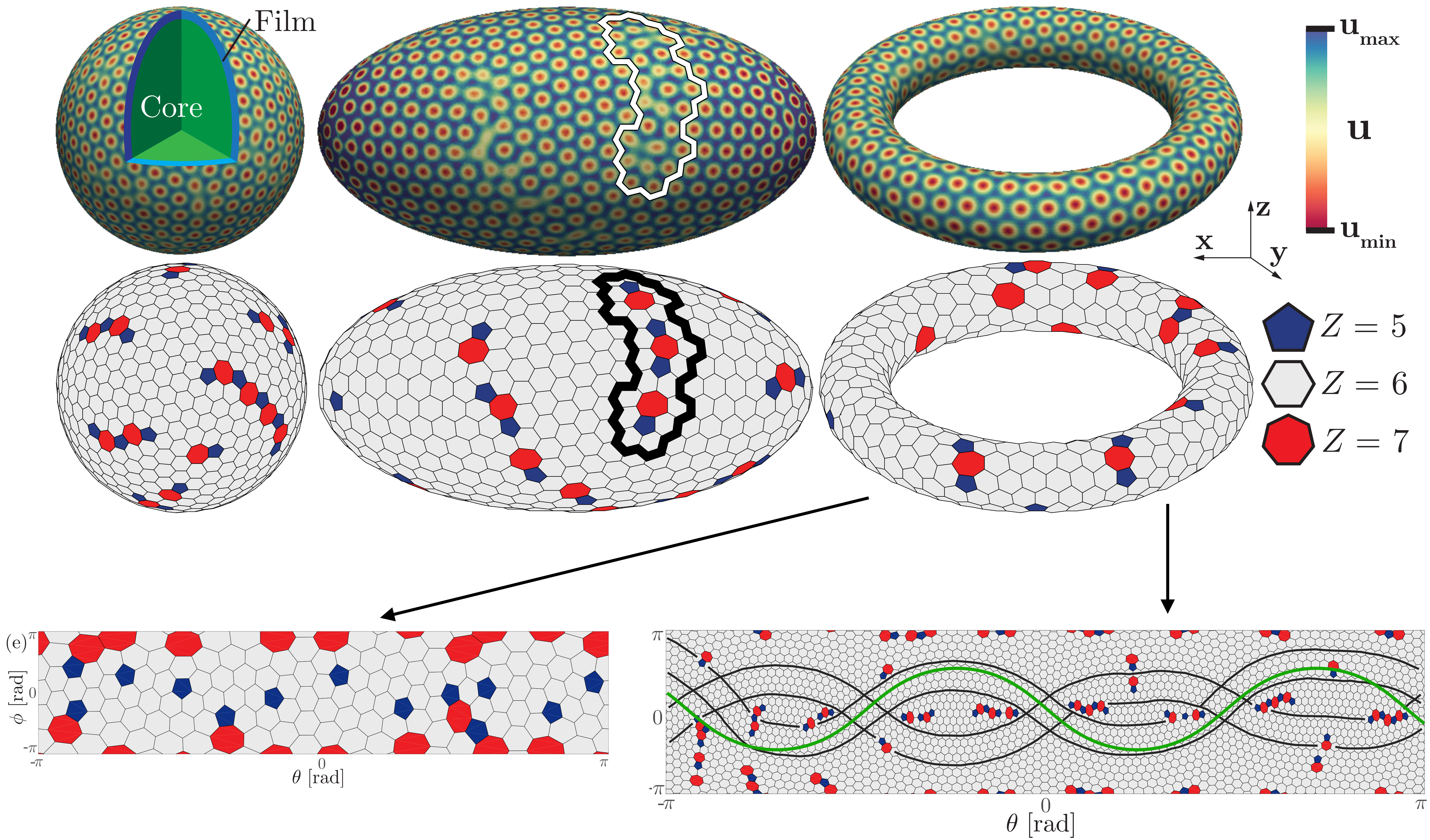
Irvine et al (2010) Nature

Nucleation



Meng, Paulose, Nelson & Manoharan (2014) Science

Statics: surface crystallography

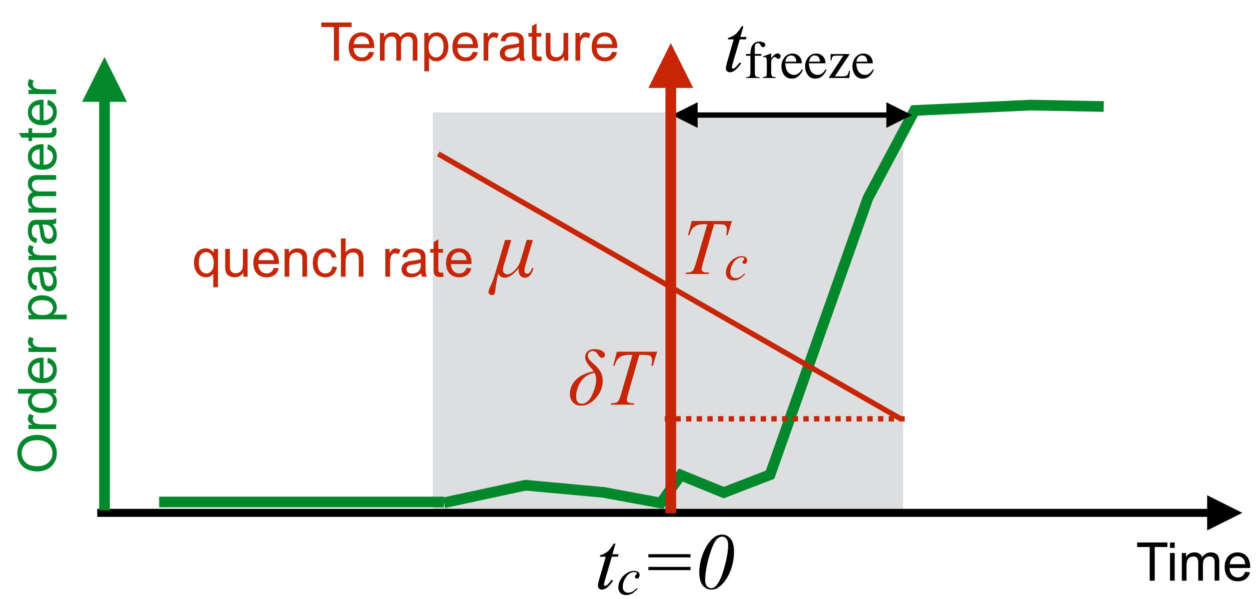


PRL 2016 (joint work with Reis lab MIT MechE)

Dynamics: Kibble-Zurek mechanism (KZM)

Kibble & Zurek (1970s): System driven through a 2nd order phase transition

- exhibits critical slowing-down
- dynamics cannot follow changes of external system parameters
- density of topological defects after quench reveals information about the quench dynamics
- observed topological structures in the universe provide a window into early evolution

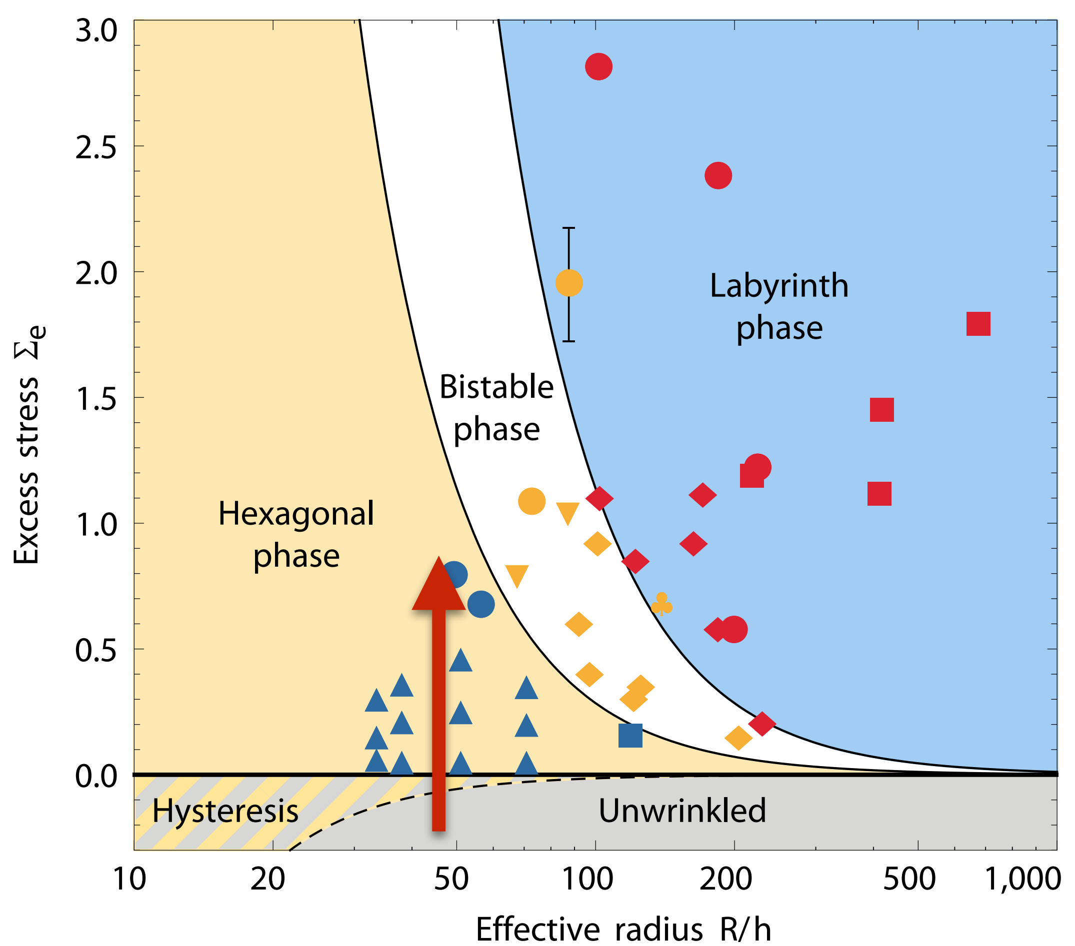


KZ predictions:

$$T(t) = T_c - \mu t \;\Rightarrow\; t_{\text{freeze}} \sim \mu^{-1/2}$$

$$\delta T(t_{\text{freeze}}) \sim \mu^{1/2}$$

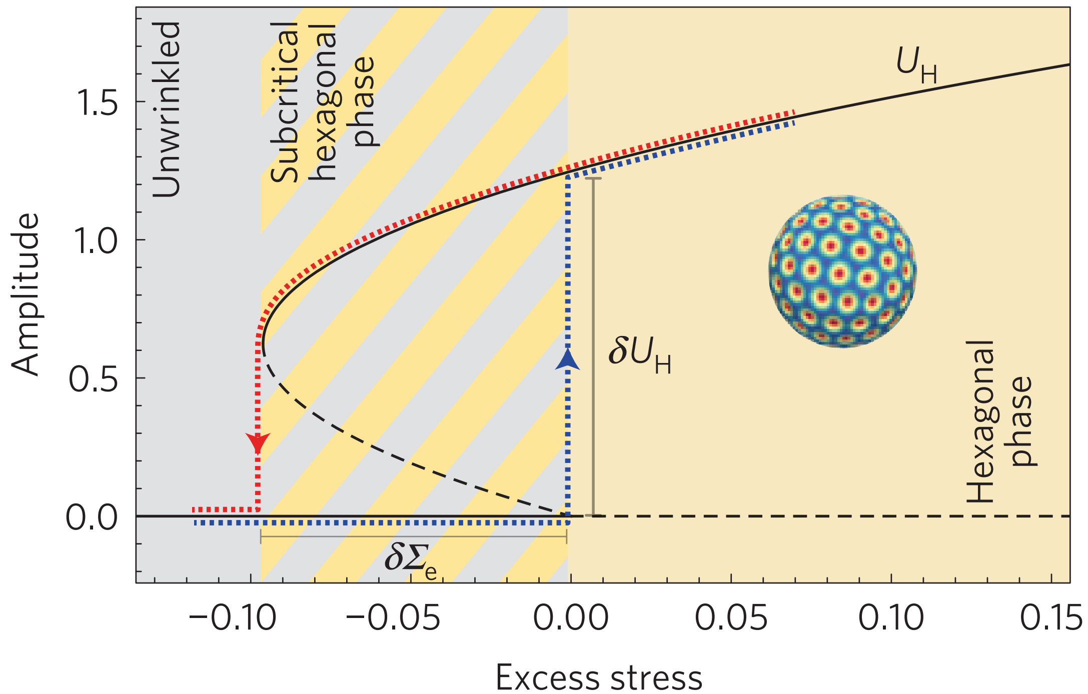
$$\rho_{\text{defect}} \sim \mu^{1/2}$$



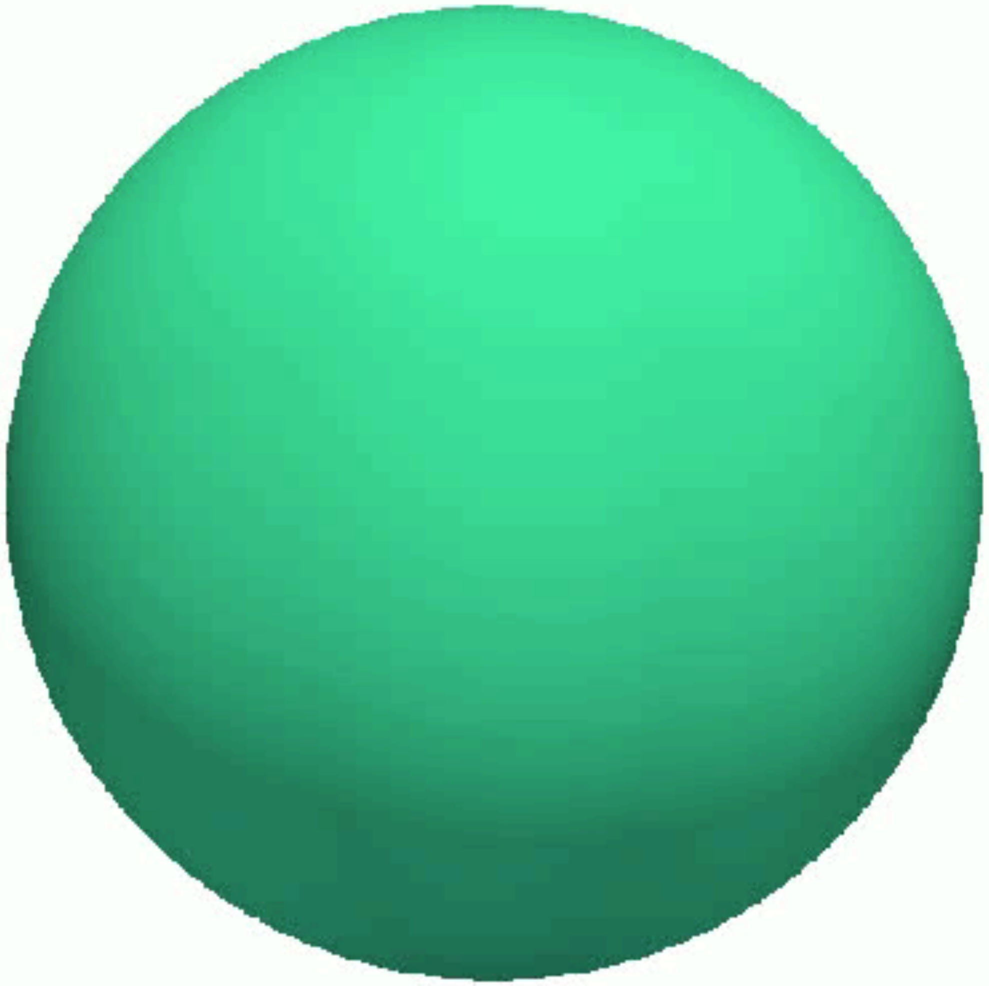
Elastic surface crystals as testbed for KZM in curved geometries?

Dynamics of phase transition

Adiabatic/equilibrium



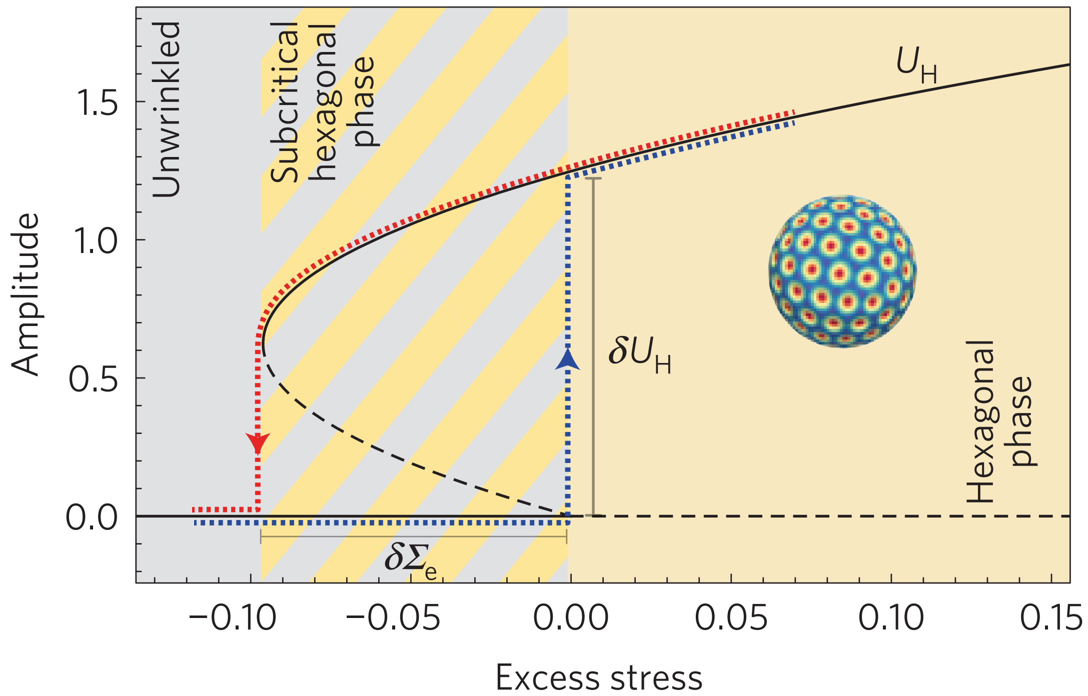
bifurcation from flat state $u=0$
to hexagonal pattern at $\Sigma_e = 0$



Stoop & Dunkel
arXiv:1703.03540

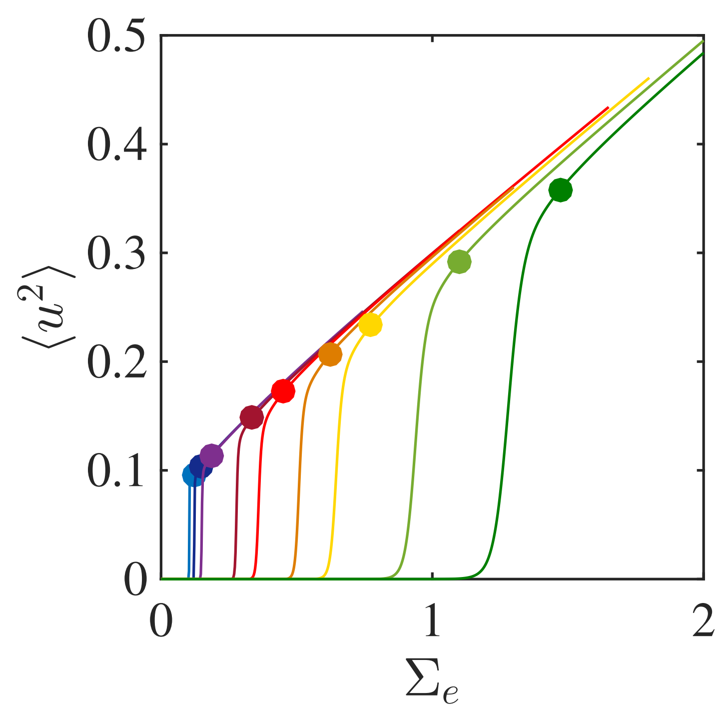
Freeze-out time follows KZ scaling

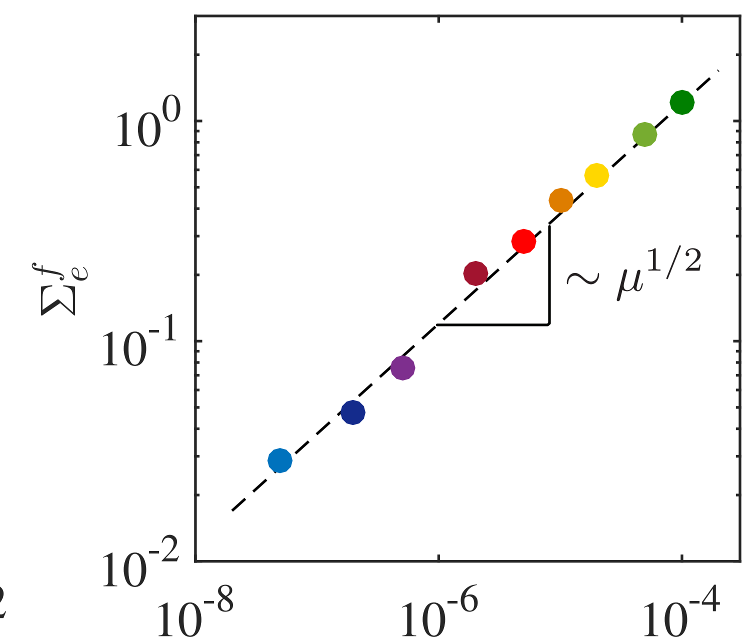
Adiabatic/equilibrium



bifurcation from flat state u=0
to hexagonal pattern at Σ_e=0

Linear quench $\Sigma_e(t) = \mu t$





$$\Sigma_e^f \sim \mu^{1/2}$$

Stoop & Dunkel
arXiv:1703.03540

Freeze-out time follows KZ scaling

$$u(t,\mathbf{x}) = U(t)\sum_{a=1}^{3}\left(e^{i\mathbf{k}_a\cdot\mathbf{x}} + e^{-i\mathbf{k}_a\cdot\mathbf{x}}\right)$$

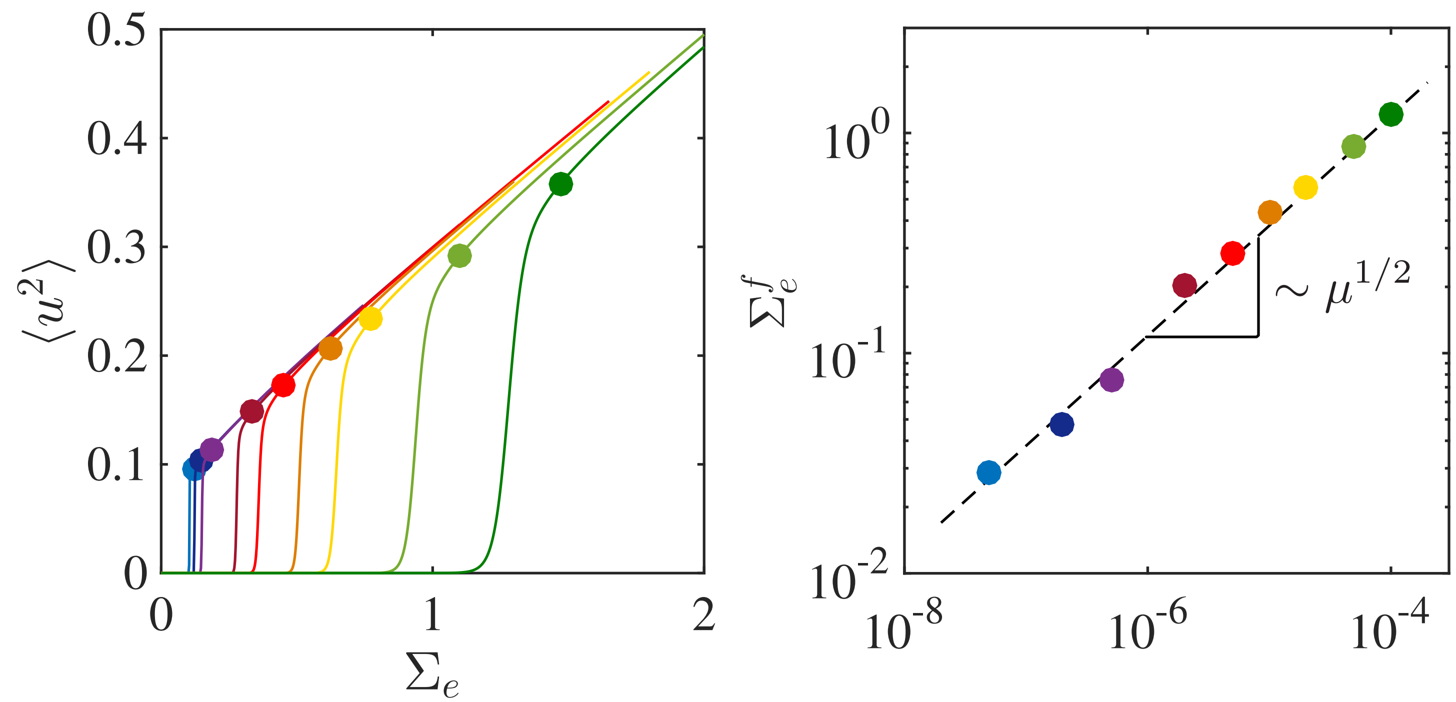
$$\frac{dU}{dt} = \frac{c\Sigma_e}{12\gamma_0^4}U - \frac{4}{3R|\gamma_0|^3}U^2 - \frac{15c}{9\gamma_0^4}U^3$$

$$\frac{d}{dt}U \approx \frac{c\mu t}{12\gamma_0^4}U$$

$$t' = \mu^{1/2}t$$

$$\frac{d}{dt'}U \approx \frac{ct'}{12\gamma_0^4}U$$

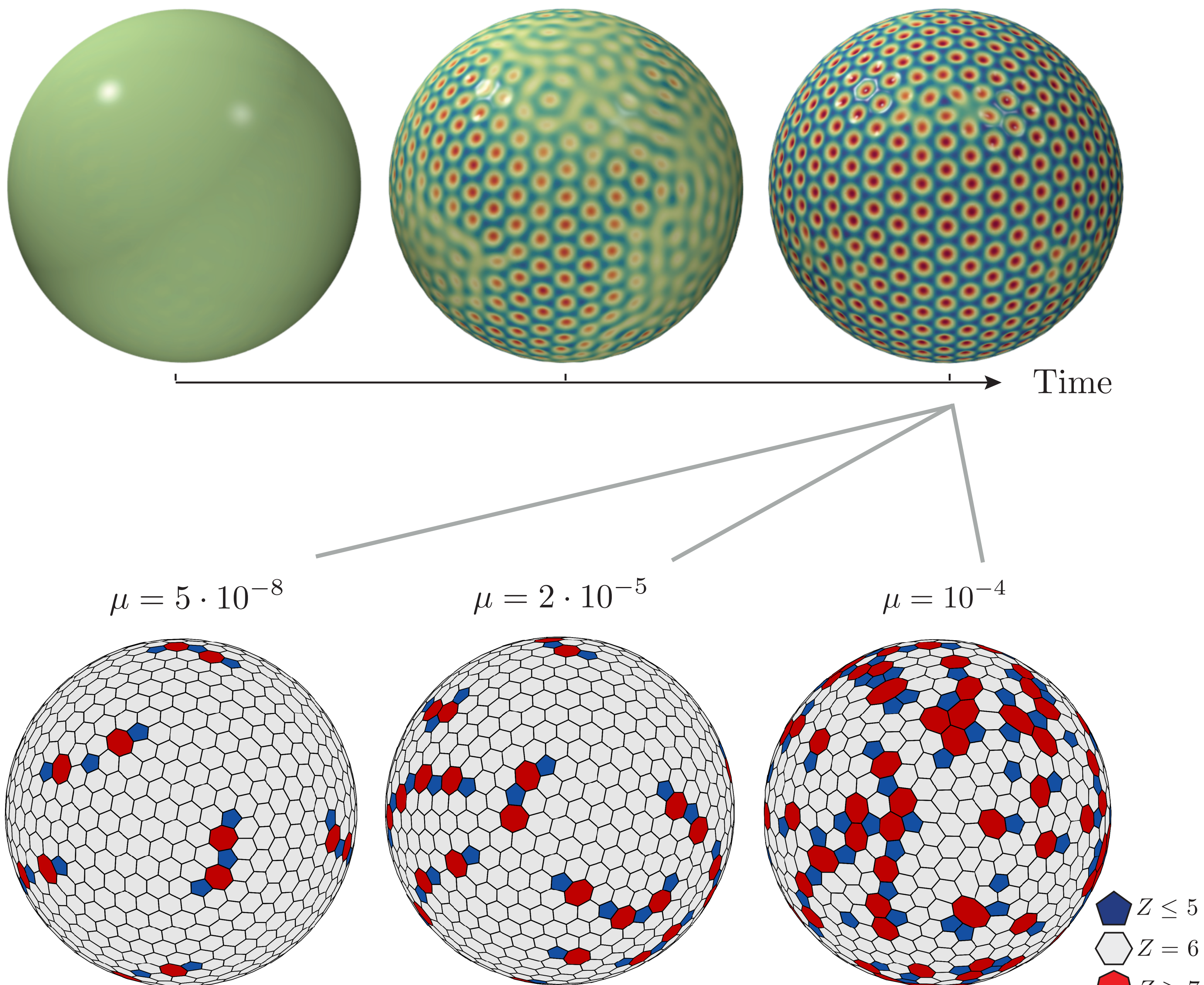
Linear quench $\Sigma_e(t) = \mu t$



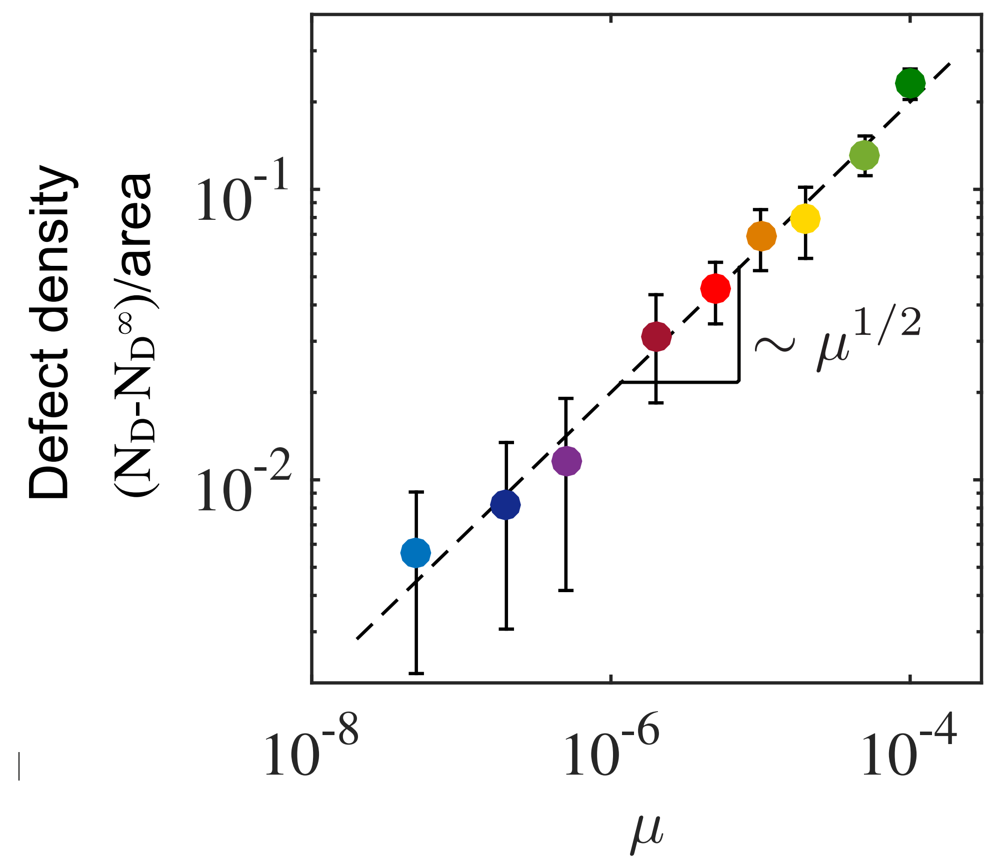
$$\Sigma_e^f \sim \mu^{1/2}$$

Stoop & Dunkel
arXiv:1703.03540

Defect density follows KZ predictions !?



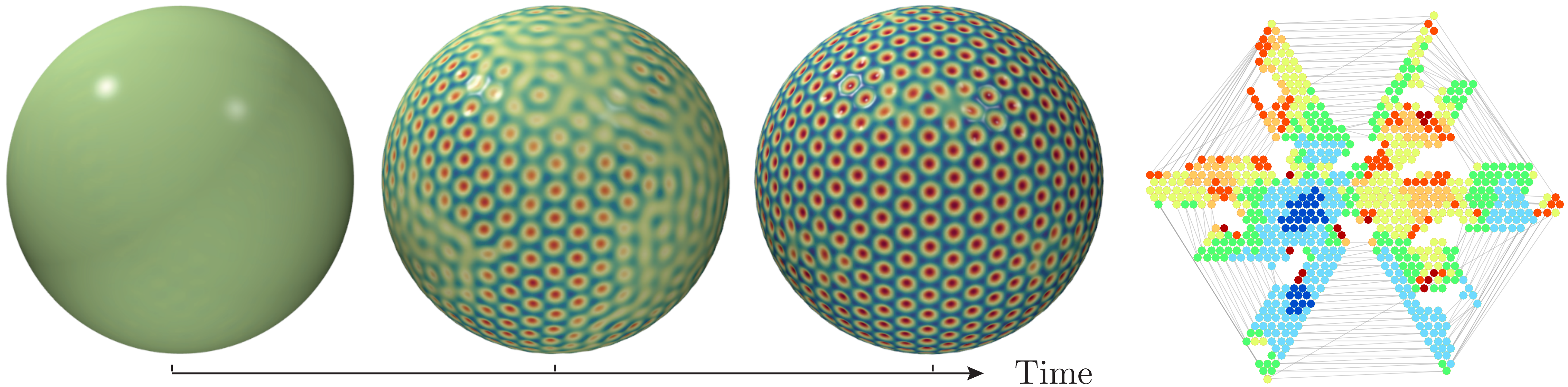
Voronoi tessellation at freeze-out $\boldsymbol{\Sigma_e^f}$

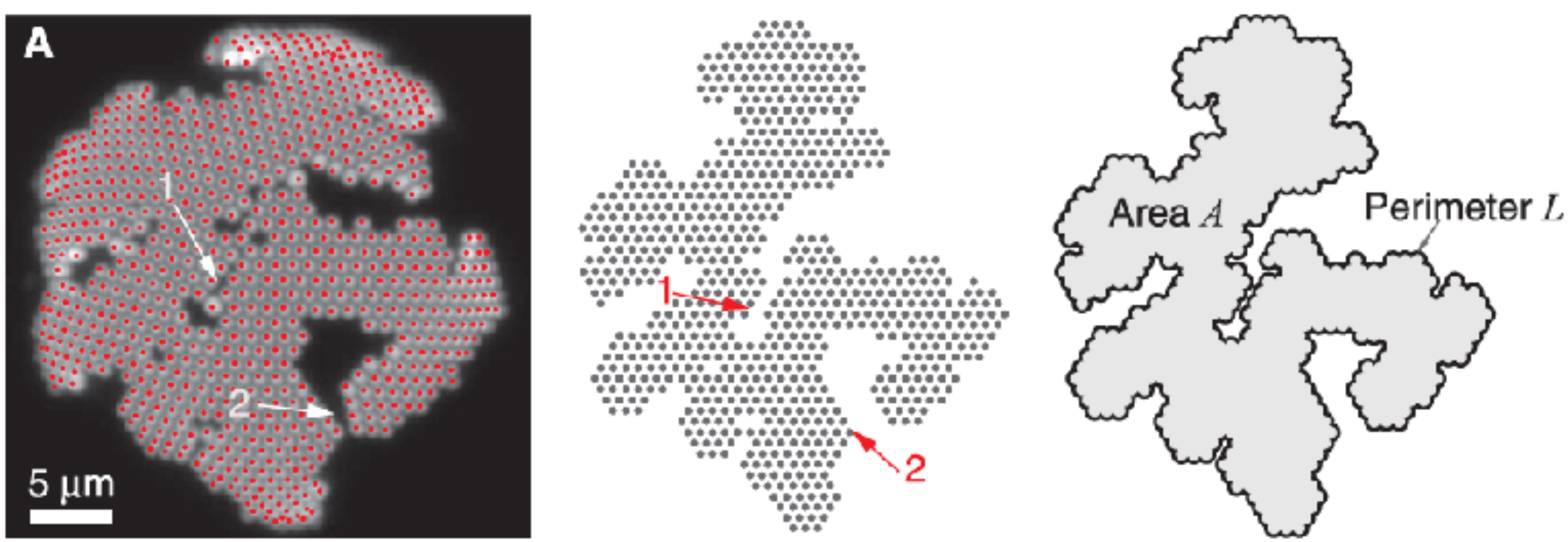


$$\rho_{\text{defect}} \sim \mu^{1/2}$$

Stoop & Dunkel (2016) Preprint

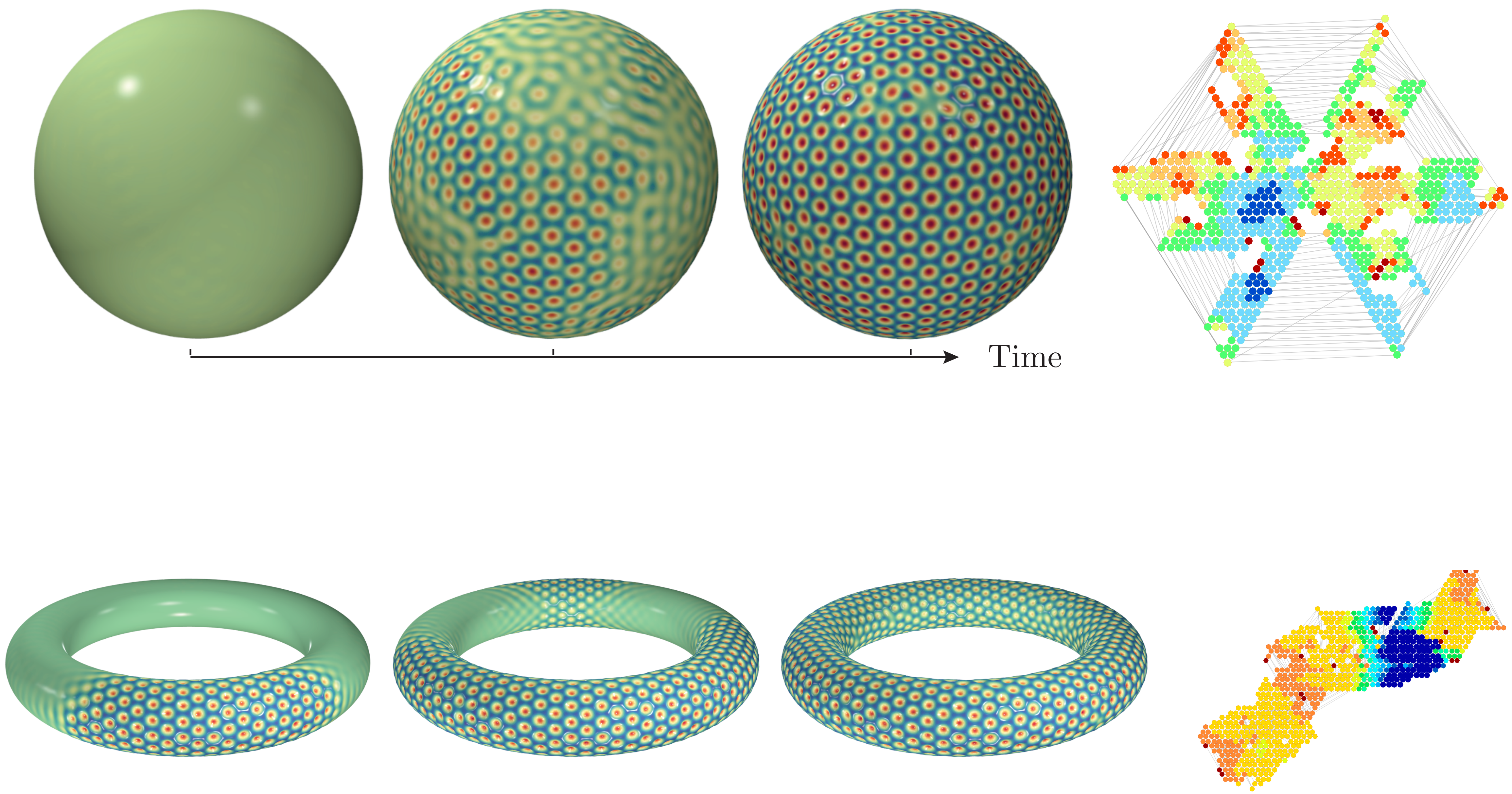
Nucleation dynamics



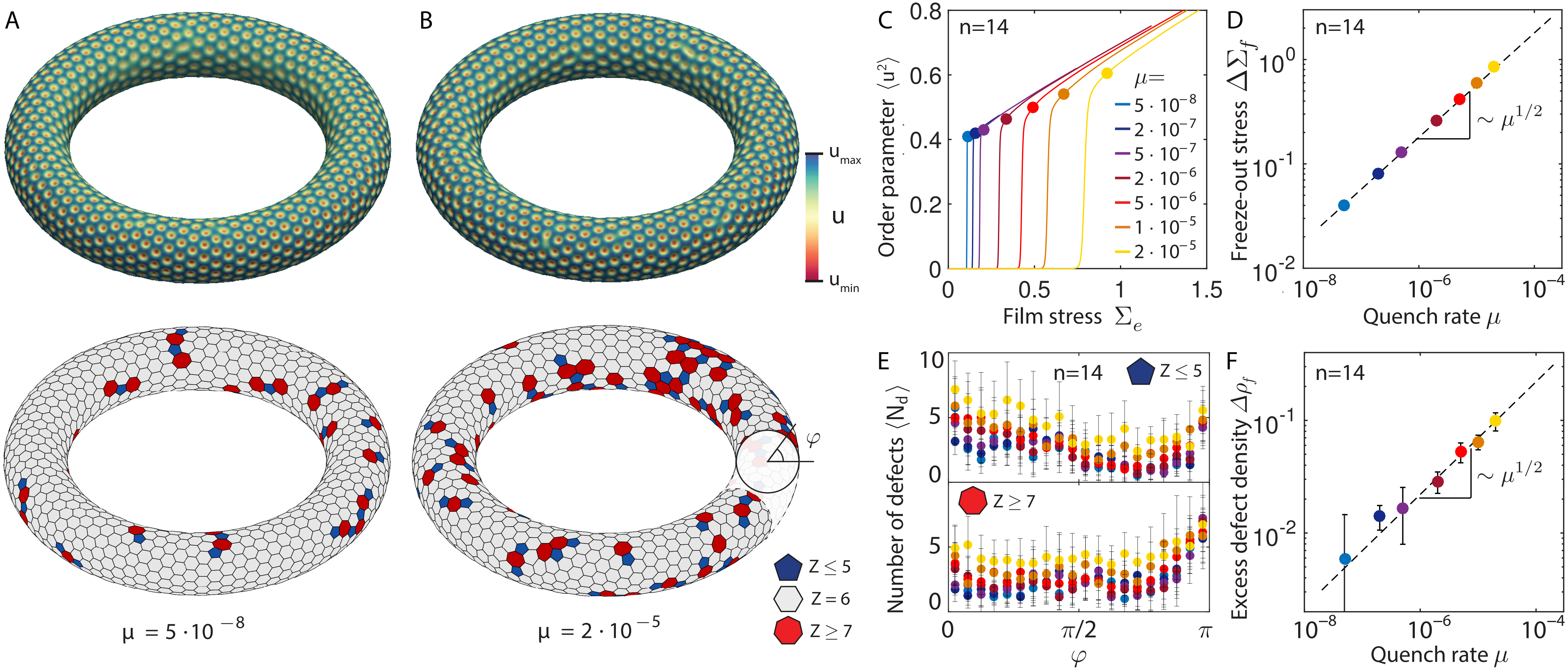


Meng, Paulose, Nelson & Manoharan (2014) Science

Nucleation dynamics



explains 'geodesic wrapping'



Stoop & Dunkel
arXiv:1703.03540