An effective model for the wrinkling of elastic bilayer systems

KITP, 2015

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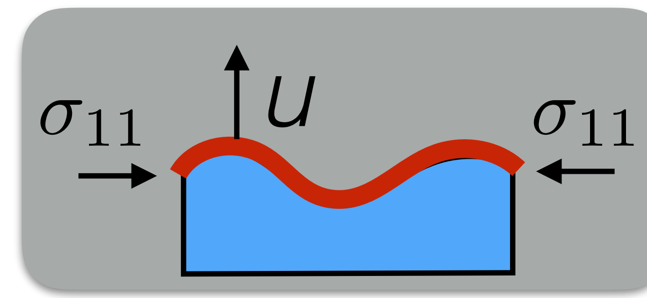
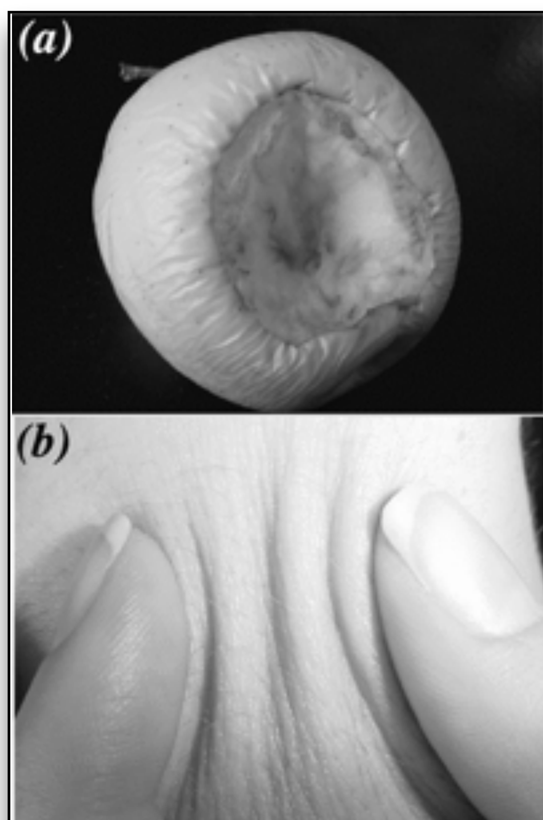
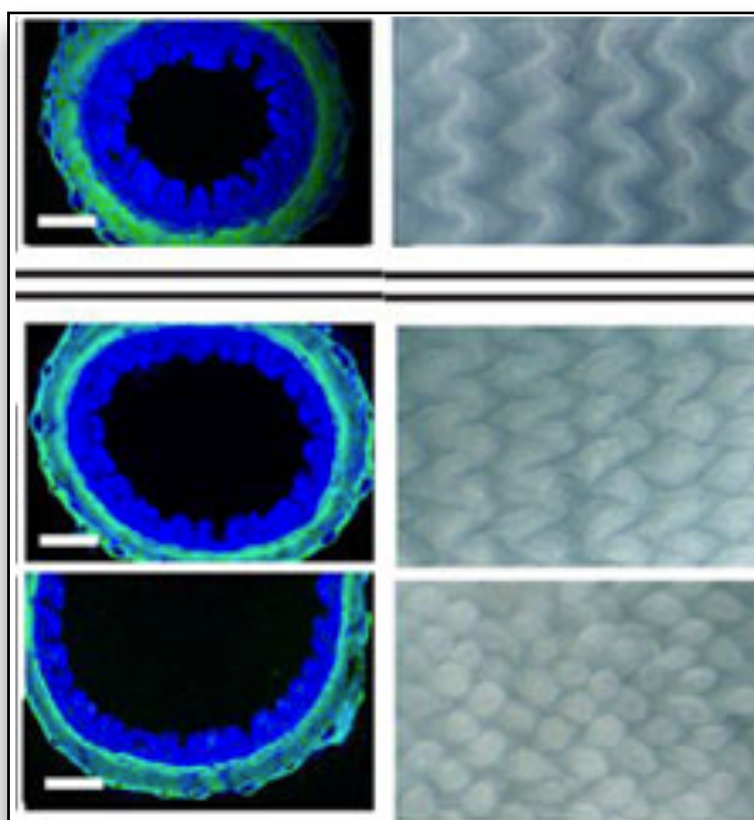
MIT Dept. of Mathematics

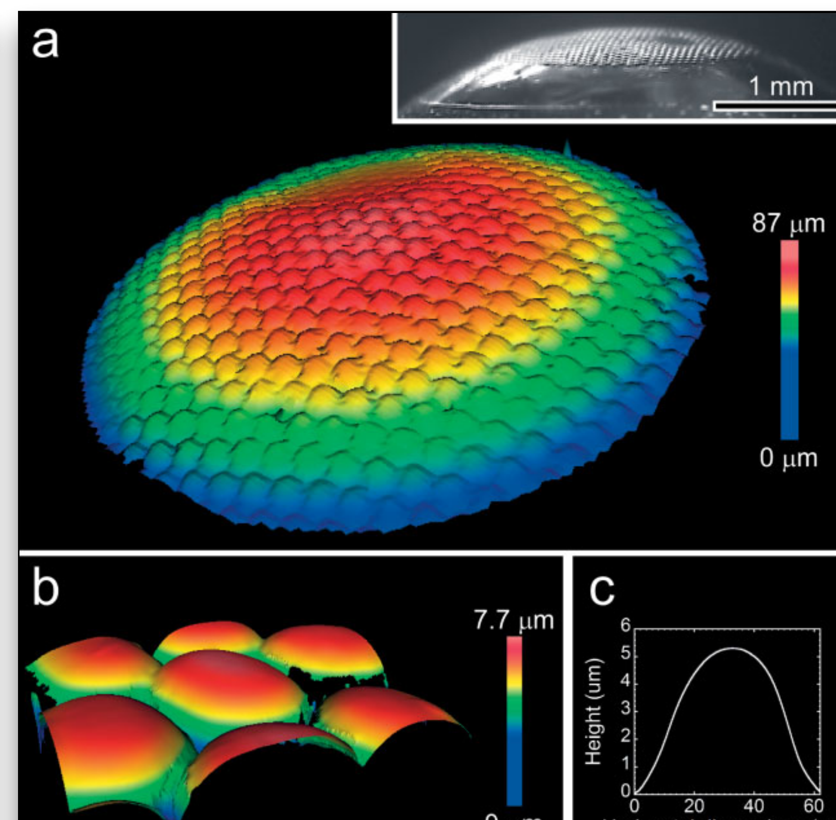




E. Cerda et al, PRL, 2003

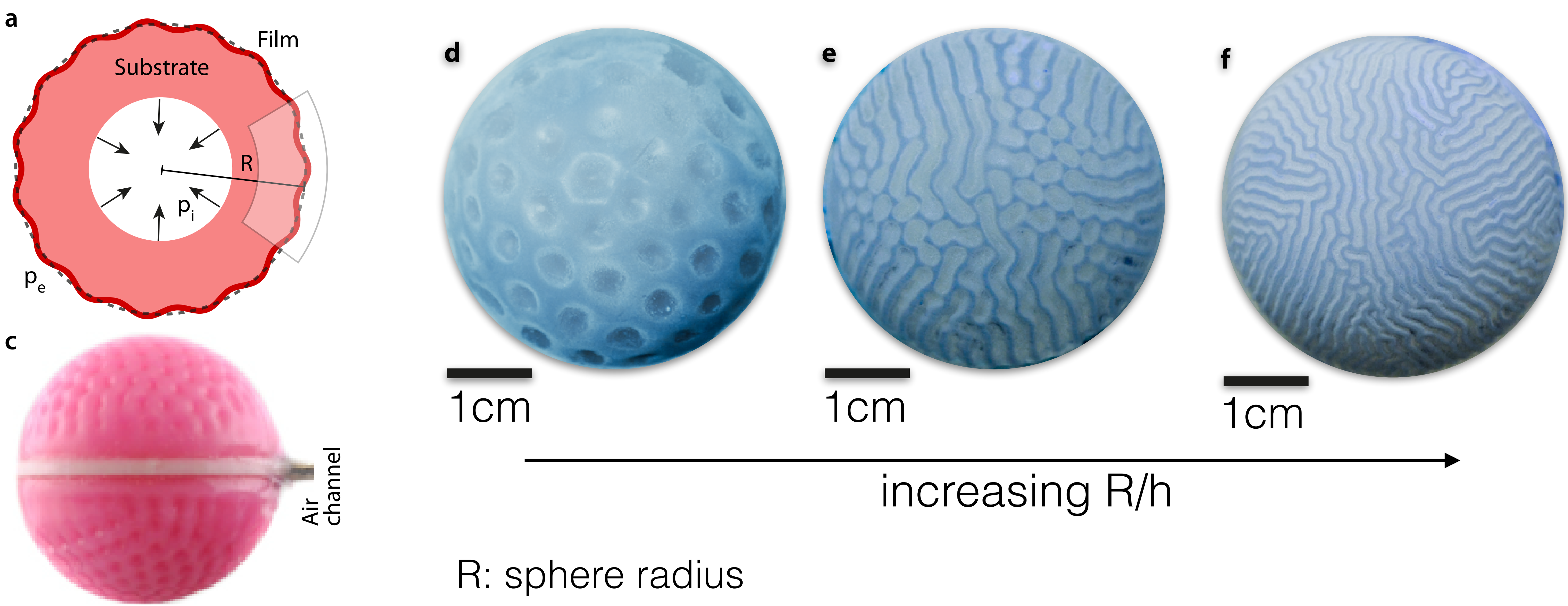


A.E. Shyer et al, Science 2013



E.P. Chan, Adv. Mat. 2006

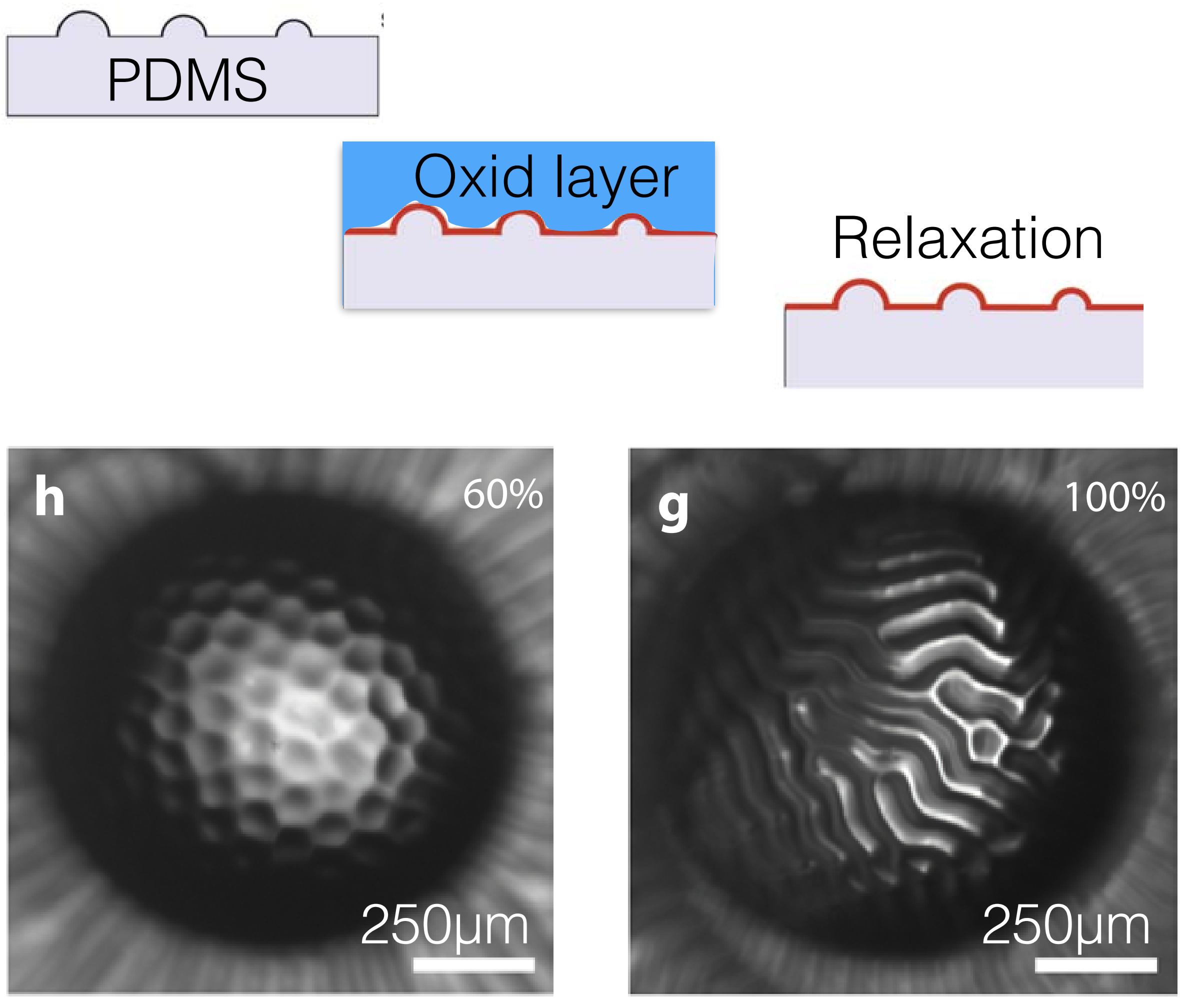
Curvature-induced phase transition



D. Terwange et. al., Adv. Mat. 2014

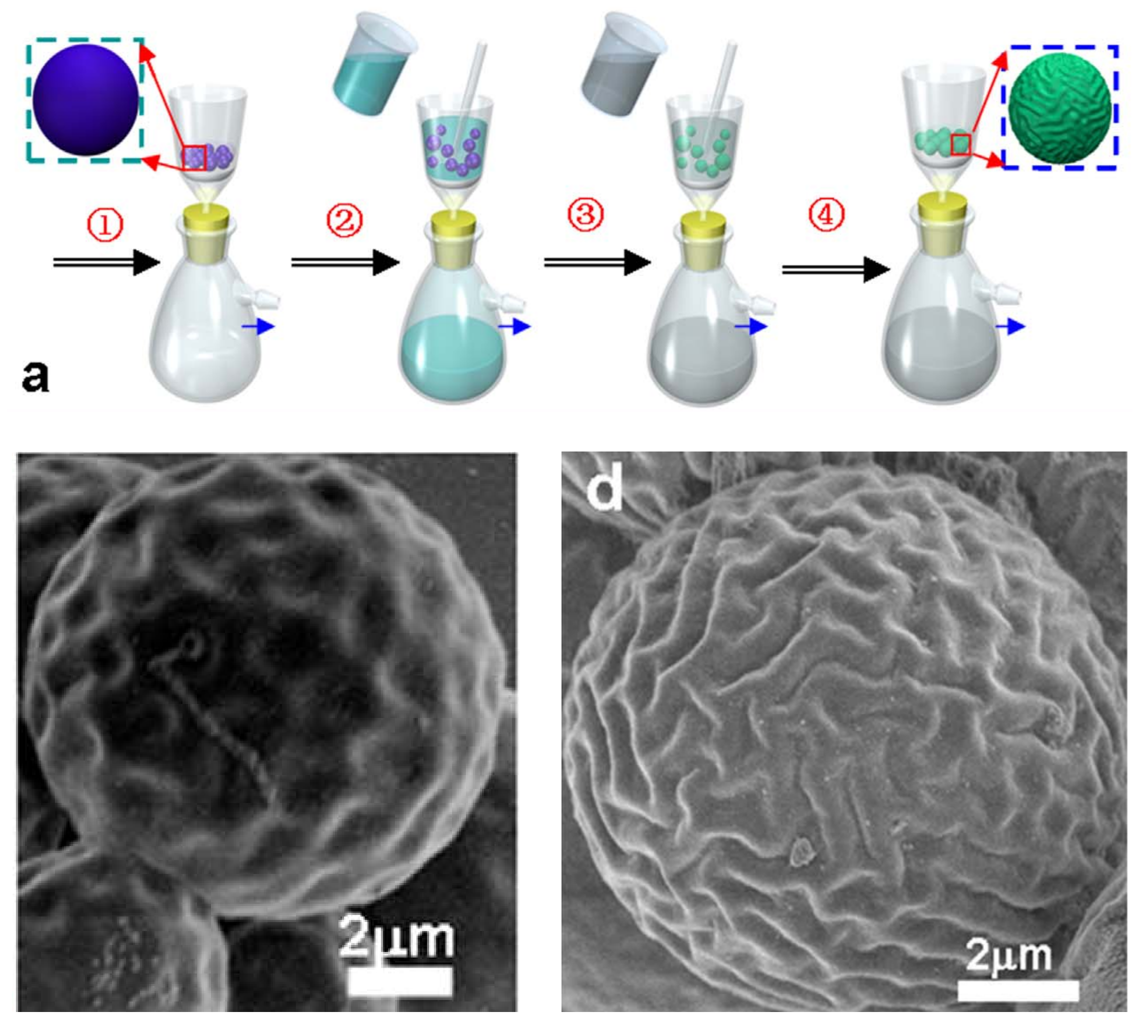
R: sphere radius
h: film thickness

Influence of film stress



Increasing film stress

D. Breid et al, Soft Matter, 2013



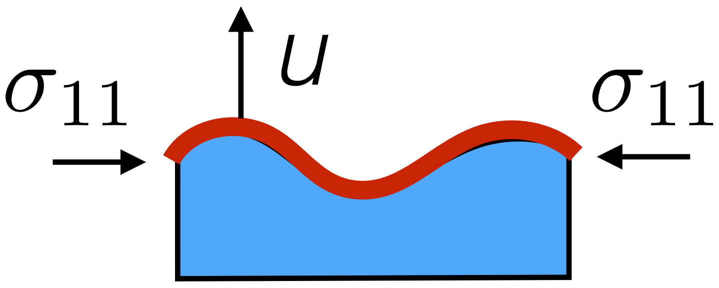
Increasing film stress

J. Yin et al, Sci. Rep., 2013

- Experiments suggest: Curvature and film stress determine wrinkling patterns

Wrinkling of thin films on substrates: Known results

- Planar case:
  System described by nonlinear Föppl-von Karman equations for normal displacement *u* and in-plane stresses $\sigma_{\alpha\beta}$



- In addition to Karman's equations, the elasticity BVP of the substrate needs to be solved.
- Difficulties:
  - Karman equations…
  - Curved substrates?

- Linear stability analysis gives critical buckling stress and wavelength:

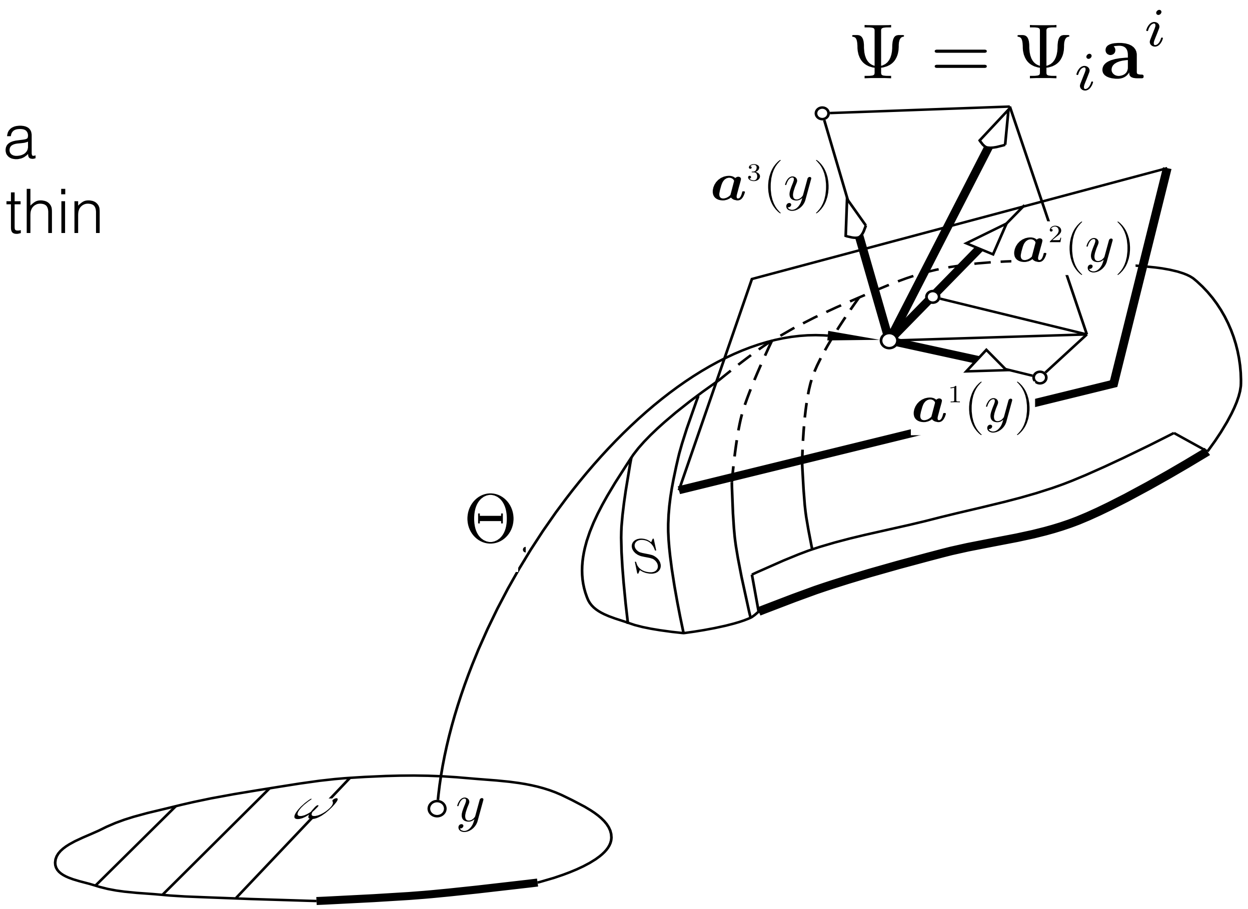
$$k_c = 2\pi/\lambda_c = \left(3\frac{E_s}{E_f}\right)^{\frac{1}{3}}$$

E_s: Substrate Young modulus
E_f: Film Young modulus

Towards an effective wrinkling theory

- We start from the Koiter shell (KS) model, a covariant formulation of the mechanics of thin films.
- Parameters and fields:

E_f	Film Young modulus
h	Film thickness
R	Substrate radius
ν	Poisson ratio
$\Psi = \Psi_i \mathbf{a}^i$	Displacement field



- The KS energy is

$$\mathcal{E}_{\mathrm{KS}}(\Psi) = \mathcal{E}_b(\Psi) + \mathcal{E}_s(\Psi) + \mathcal{E}_f(\Psi)$$

bending energy, stretching energy, ext. forces (pressure)

effective model: substrate coupling via ext. forces

Towards an effective wrinkling theory

- Bending and stretching energy are described entirely by the displacement field ψ:

$$\mathcal{E}_s = \frac{E_f}{2(1-\nu^2)} \int_\omega d\omega \, \frac{h}{2} H^{\alpha\beta\gamma\delta} G_{\gamma\delta}(\Psi) G_{\alpha\beta}(\Psi)$$

$$\mathcal{E}_b = \frac{E_f}{2(1-\nu^2)} \int_\omega d\omega \, \frac{h^3}{24} H^{\alpha\beta\gamma\delta} R_{\gamma\delta}(\Psi) R_{\alpha\beta}(\Psi)$$

- H: constitutive tensor (material law)

The stretching strains are

$$G_{\alpha\beta} = \frac{1}{2}\left[a_{\alpha\beta}(\Psi) - a_{\alpha\beta}\right]$$

deformed — undeformed

metric tensor

The bending strains are

$$R_{\alpha\beta} = b_{\alpha\beta}(\Psi) - b_{\alpha\beta}$$

deformed — undeformed

curvature tensor

- Expand Ψ in dominant part *u* (normal displacement)

Towards an effective wrinkling theory

- Bending and stretching energy are described entirely by the displacement field Ψ:

$$\mathcal{E}_s = \frac{E_f}{2(1-\nu^2)} \int_\omega d\omega \; \frac{h}{2} H^{\alpha\beta\gamma\delta} G_{\gamma\delta}(\Psi) G_{\alpha\beta}(\Psi)$$

stretching strain ($G_{\alpha\beta}(\Psi)$)
stretching stress ($H^{\alpha\beta\gamma\delta} G_{\gamma\delta}(\Psi)$)

$$\mathcal{E}_b = \frac{E_f}{2(1-\nu^2)} \int_\omega d\omega \; \frac{h^3}{24} H^{\alpha\beta\gamma\delta} R_{\gamma\delta}(\Psi) R_{\alpha\beta}(\Psi)$$

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metric tensor

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stretching
strain
stress

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deformed undeformed
curvature tensor

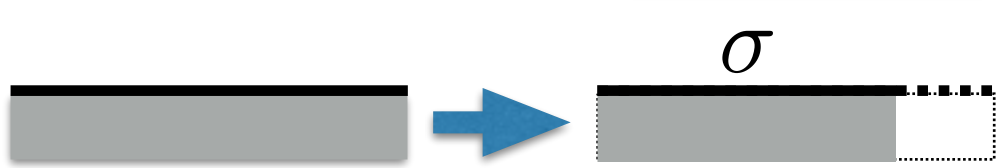
- Expand Ψ in dominant part *u* (normal displacement)

Towards an effective wrinkling theory

- Substrate energy contribution: Nonlinear spring, Young modulus E_s

$$\mathcal{E}_{sub} = \frac{E_s}{2}\int_\omega d\omega \left(\frac{\tilde{a}}{h}u^2 + \frac{\tilde{c}}{h^3}u^4\right)$$

- Excess film stress: $\Sigma_e \equiv \frac{\sigma}{\sigma_c} - 1$



$$\mathcal{E}_\sigma = \frac{E_f}{2(1-\nu^2)}\int_\omega d\omega \,\frac{\tilde{a}_2}{h}\Sigma_e u^2$$

3 unknown stiffness parameters:

$\tilde{a},\ \tilde{c}$ Effective substrate stiffness

$\tilde{a}_2 < 0$ stress-induced destiffening

Variation of total energy w.r.t. *u* gives *effective wrinkling equation*.

Effective wrinkling equation

Assuming overdamped dynamics, we obtain an effective wrinkling equation for the normal displacement field u:

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

symmetry-breaking depends on curvature:

$$b \sim \frac{1}{R^3} \quad \Gamma_1 \sim \frac{1}{R}$$

b, Γ_1: break symmetry u → -u

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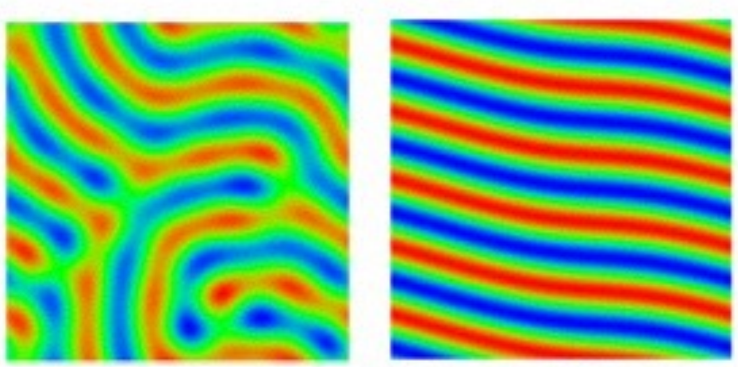
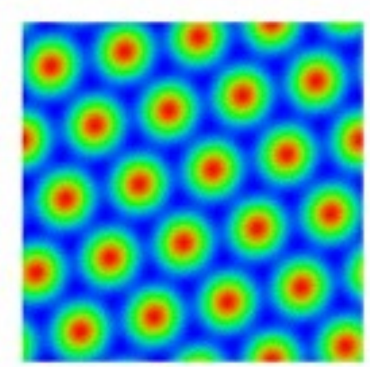
First line (planar case): Swift-Hohenberg equation (Rayleigh-Bénard convection)

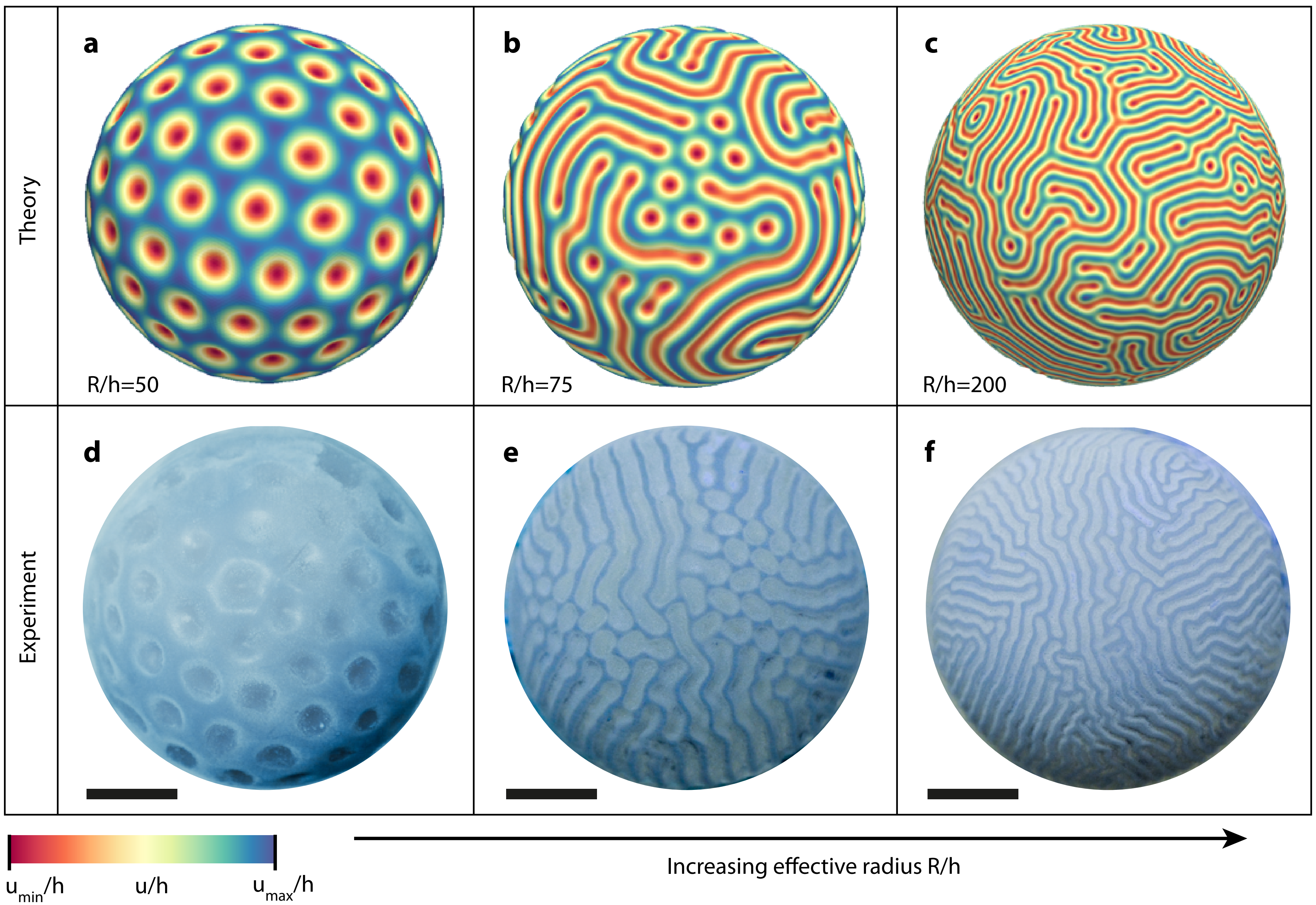


sym.breaking coefficients = 0



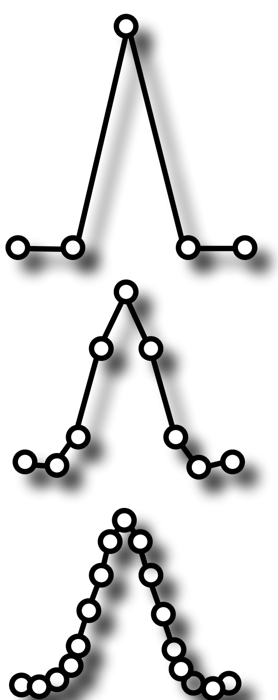
sym.breaking coefficients > 0

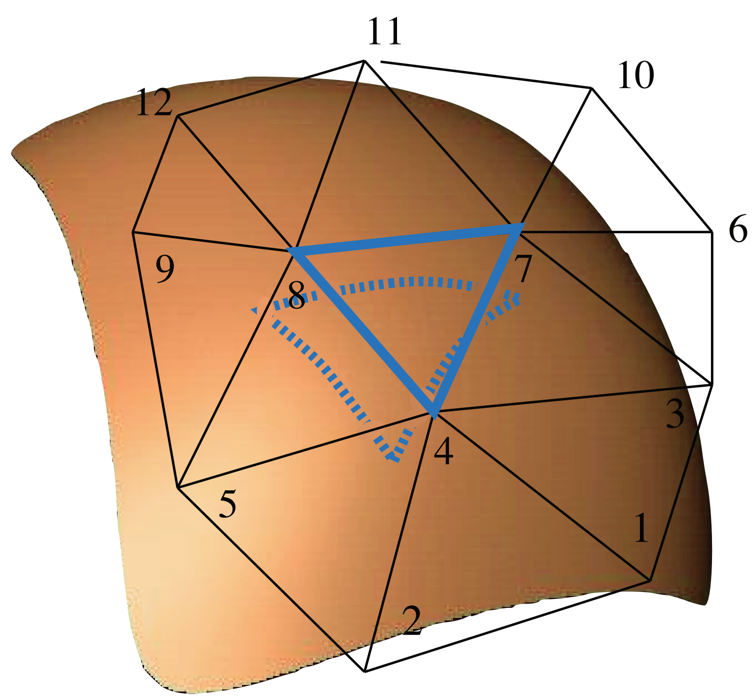
Numerical results



A word about numerics…

- Need to solve covariant, 4th order PDE on a surface…
- Use a spline-based Finite Element method (Cirak, 2001):





- Limit of infinitely many subdivisions (J. Stam, 1966):

$$\mathbf{x}(\theta^1, \theta^2) = \sum_{I=1}^{12} N^I(\theta^1, \theta^2)\mathbf{x}_I$$

- N^I: quartic spline functions

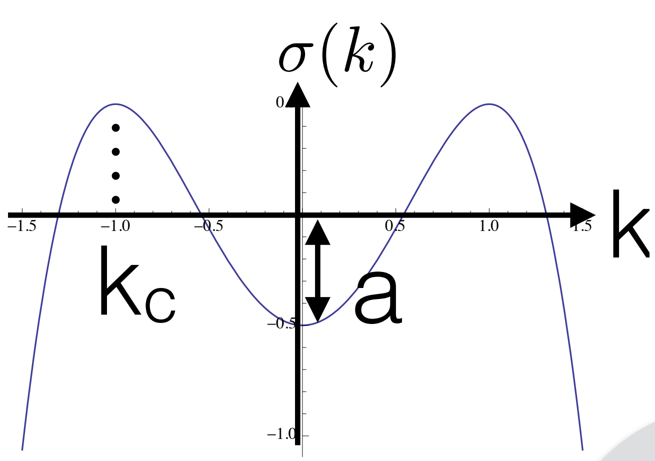
Wavelength and stiffness matching

Wrinkling equation: $\partial_t u = \gamma_0 \Delta u - \gamma_2 \Delta^2 u - au - bu^2 - cu^3$

$$+ \Gamma_1 \left[(\nabla u)^2 + 2u\Delta u \right] + \Gamma_2 \left[u(\nabla u)^2 + u^2 \Delta u \right]$$

Undetermined: γ_0 and 3 effective stiffness parameters (in parameters a and c).

Asymptotic matching in the planar case R->∞ : Perturb unwrinkled state u=0 with plane waves $\epsilon e^{ikx+\sigma t}$



Wavelength: $|k| = \sqrt{\frac{|\gamma_0|}{2\gamma_2}}$ ⟺ classical wrinkling: $k_c = \left(3\frac{E_s}{E_f}\right)^{\frac{1}{3}}$

=> determines γ_0

Bifurcation condition:

$$a = \frac{\gamma_0^2}{4\gamma_2} = \frac{1}{12}\left(\frac{3E_s}{E_f}\right)^{4/3}$$

=> linear substrate stiffness

Amplitude law for wrinkles:

$$\epsilon/h = \sqrt{\Sigma_e}$$

=> stress destiffening constant

=> one fit parameter (appearing in c) remains undetermined

Parameters

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

Geometry & material parameters

$\eta = 3E_s/E_f$

$\gamma_2 = 1/12$

$\Sigma_e = (\sigma/\sigma_c) - 1$

$\kappa = h/R$

One free fit parameter c_1

$$\gamma_0 = \frac{\kappa^2}{3} - \frac{1}{6}\sqrt{\eta^{4/3} + 24(1+\nu)\kappa^2 + 16\kappa^4}$$

$$a = \frac{\eta^{4/3}}{12} + \frac{6(1+\nu) - \eta^{2/3}}{3}\kappa^2 + \frac{\kappa^4}{3} + \tilde{a}_2 \Sigma_e$$

$$b = 3(1+\nu)\kappa^3$$

$$c = \frac{2(1+\nu)\eta^{2/3}}{3} c_1 + (1+\nu)\kappa^4$$

$$\Gamma_1 = \frac{1+\nu}{2}\kappa$$

$$\Gamma_2 = \frac{1+\nu}{2}\kappa^2$$

$$\tilde{a}_2 = -\frac{\eta^{4/3}(c + 3|\gamma_0|\Gamma_2)}{48\gamma_0^2}$$

Understanding curvature-induced pattern transition

$$\partial_t u = \gamma_0 \Delta u - \gamma_2 \Delta^2 u - au - bu^2 - cu^3$$
$$+ \mathit{\Gamma}_1 \left[(\nabla u)^2 + 2u\Delta u\right] + \mathit{\Gamma}_2 \left[u(\nabla u)^2 + u^2 \Delta u\right]$$

- Approximate $\mathit{\Gamma}_1$ and $\mathit{\Gamma}_2$ terms by average quadratic and cubic forces.
- We obtain a standard Swift-Hohenberg equation for wrinkling:

$$\partial_t u = \gamma_0 \triangle u - \gamma_2 \triangle^2 u - au - \left(b + \Gamma_1 k_c^2\right) u^2 - \left(c + \frac{\Gamma_2 k_c^2}{2}\right) u^3$$

- (Known) nonlinear stability analysis predicts phase transition lines:

Hexagonal phase:	$-\kappa^2/(20c_1^2) < \Sigma_e < \kappa^2/c_1^2$
Bistable phase:	$\kappa^2/c_1^2 < \Sigma_e < 4\kappa^2/c_1^2$
Labyrinth phase:	$4\kappa^2/c_1^2 < \Sigma_e$

$\Sigma_e = (\sigma/\sigma_c) - 1$

$\kappa = h/R$

c_1 : fit parameter

Phase & bifurcation diagram

- Nonlinear stability analysis predicts phase transition lines:

Hexagonal phase:	$-\kappa^2/(20c_1^2) < \Sigma_e < \kappa^2/c_1^2$
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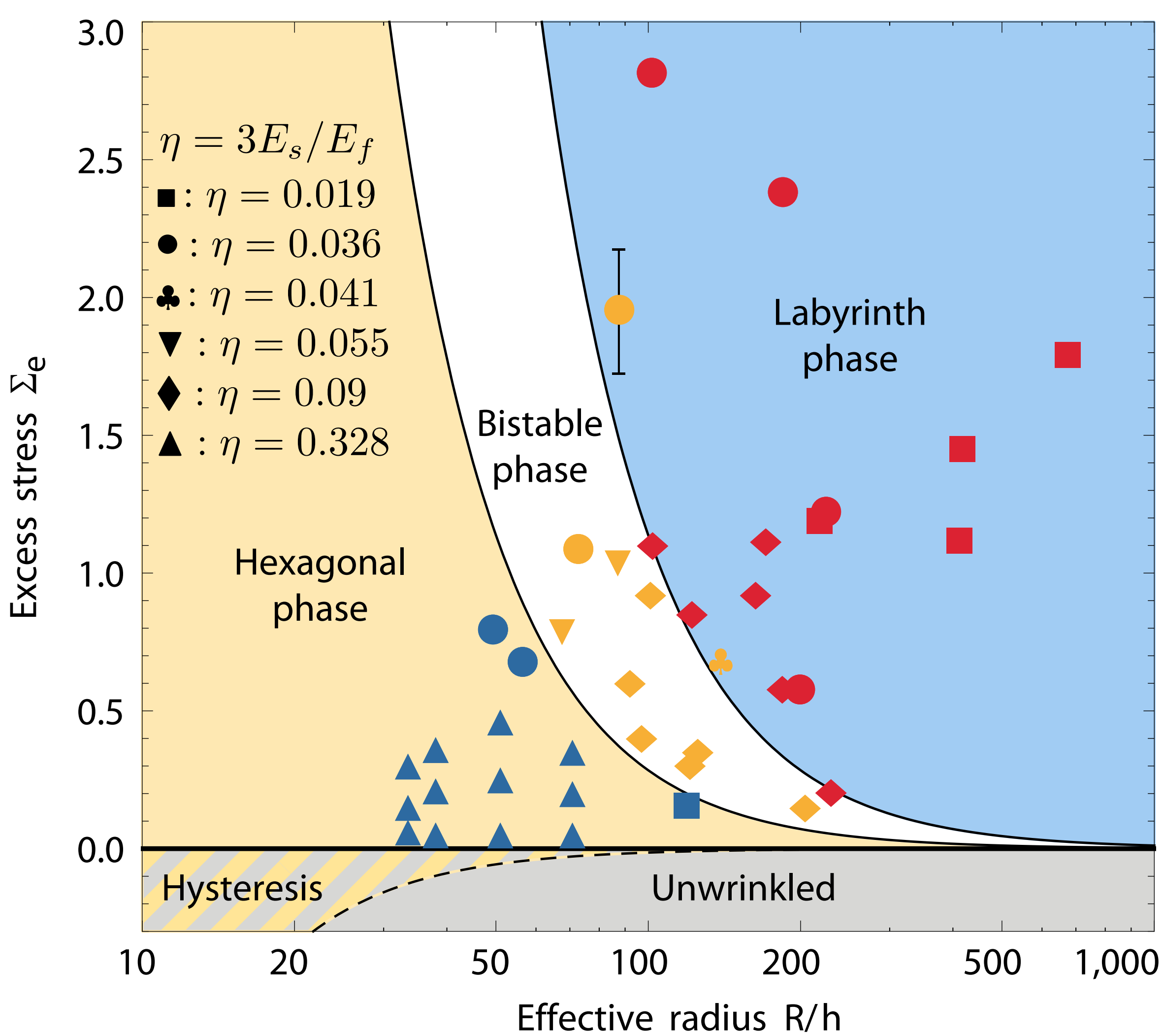
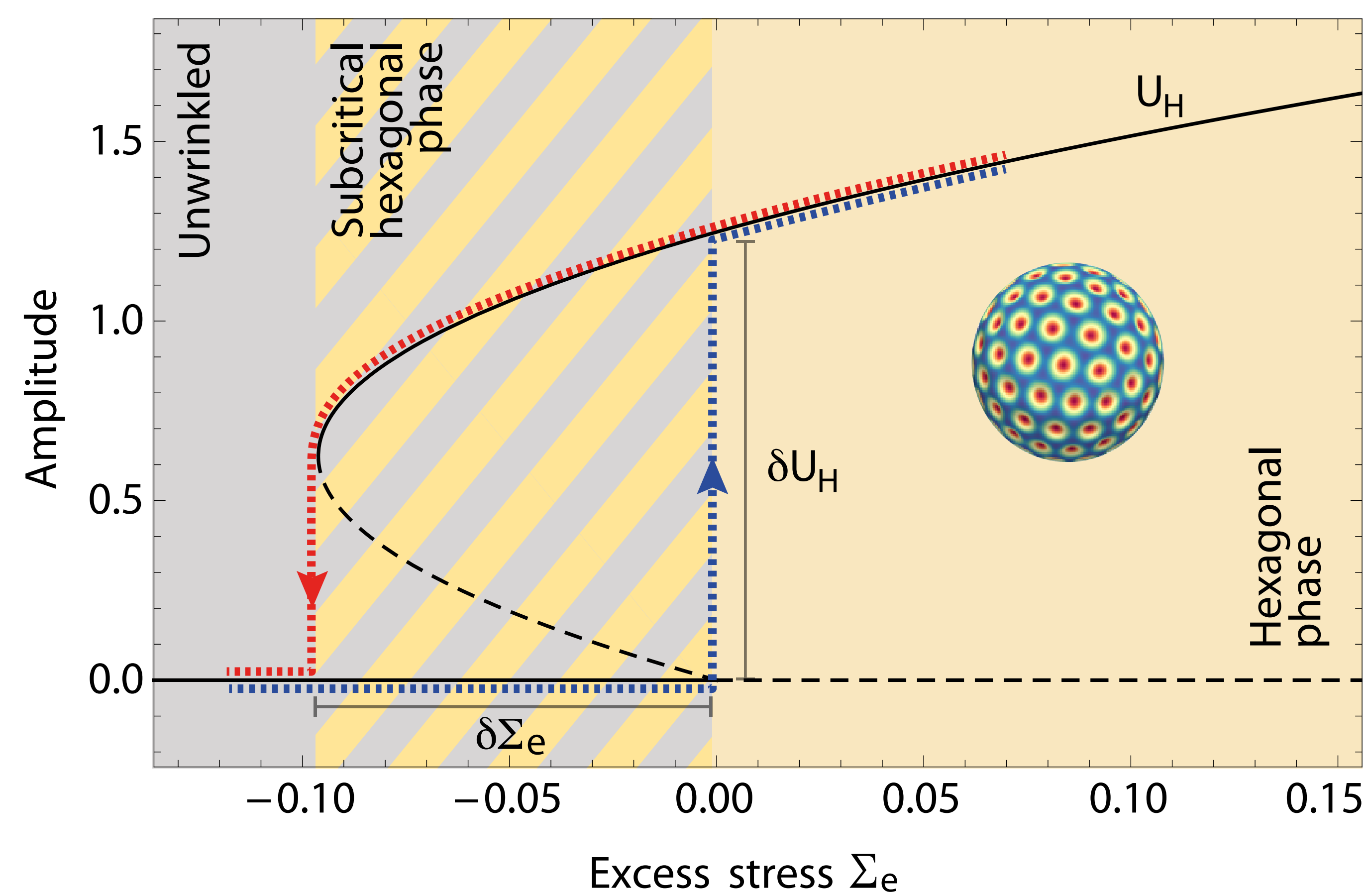
$\kappa = h/R$

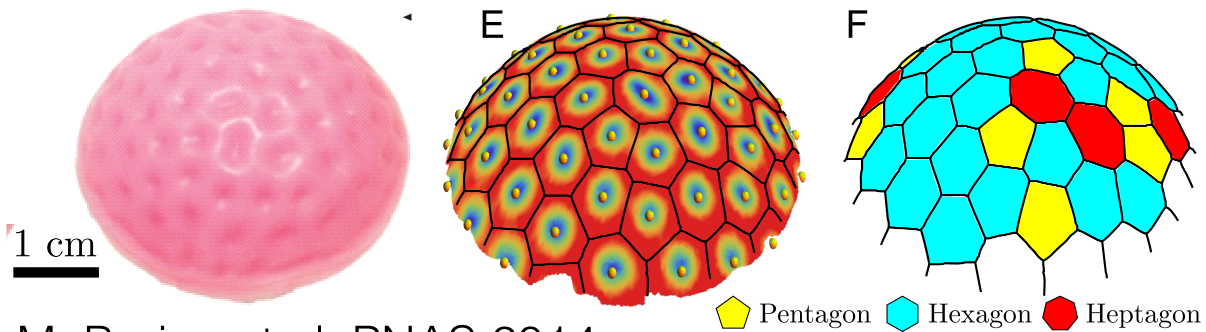
c_1 : fit parameter





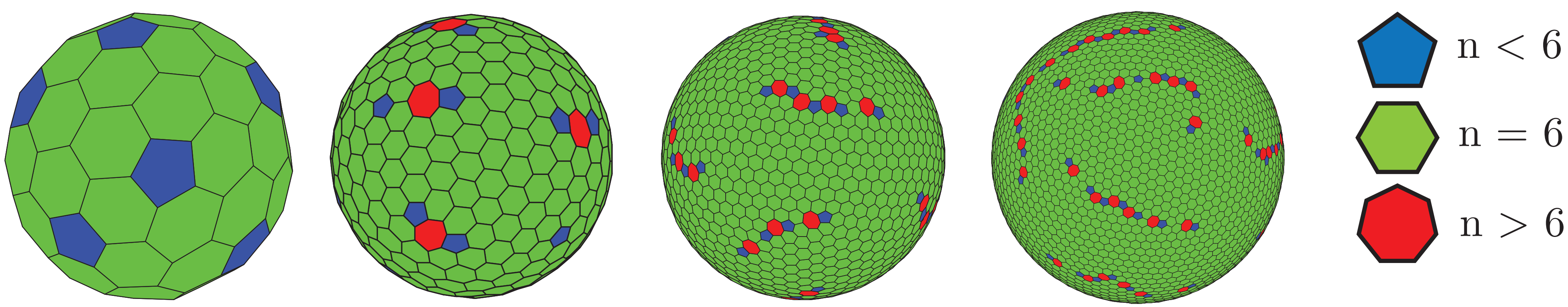
Possibility to stabilize hexagonal patterns via hysteresis?

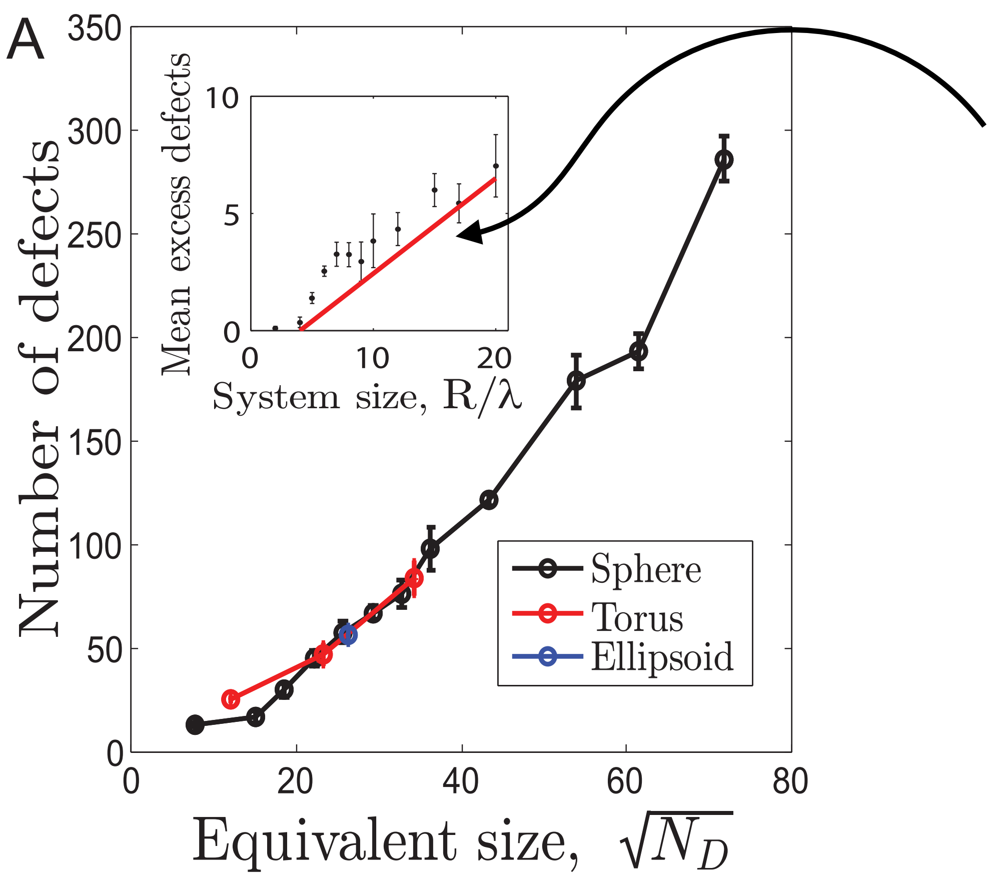
Wrinkling - a model to study curved crystals?



M. Brojan et al. PNAS 2014

Bilayer systems can be produced for (almost) arbitrary geometries => experimental testbed for curved crystals?





scaling prediction for scar length:

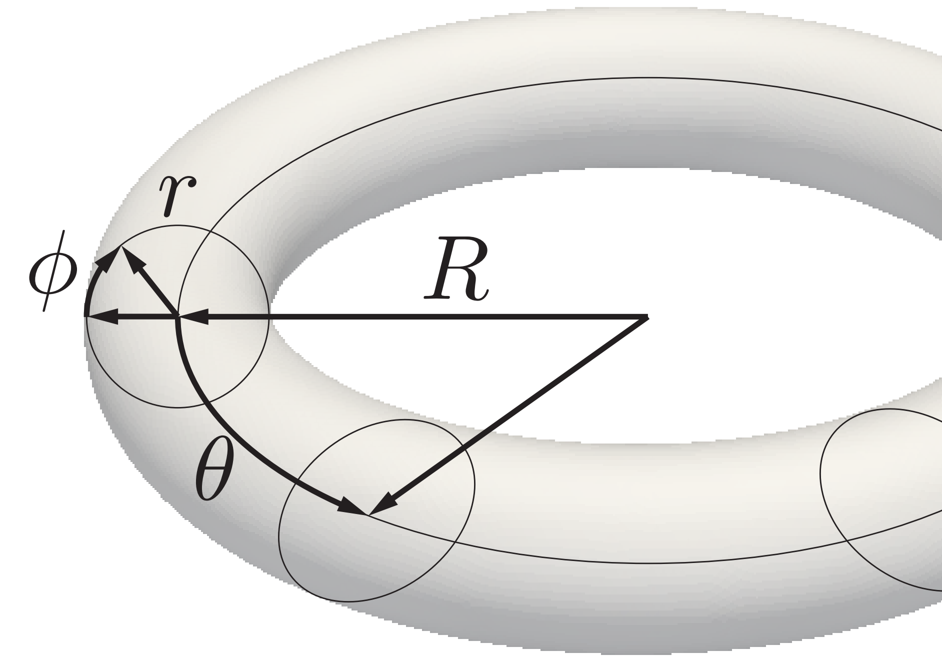
(M. Bowick, D. Nelson, and A. Travesset, Phys. Rev. B 62, 8738, 2000)

$$(\pi/3)[\sqrt{11} - 5\cos^{-1}(5/6)]R/\lambda$$

Arbitrary closed surfaces & tori

- Effective theory for arbitrary geometries:

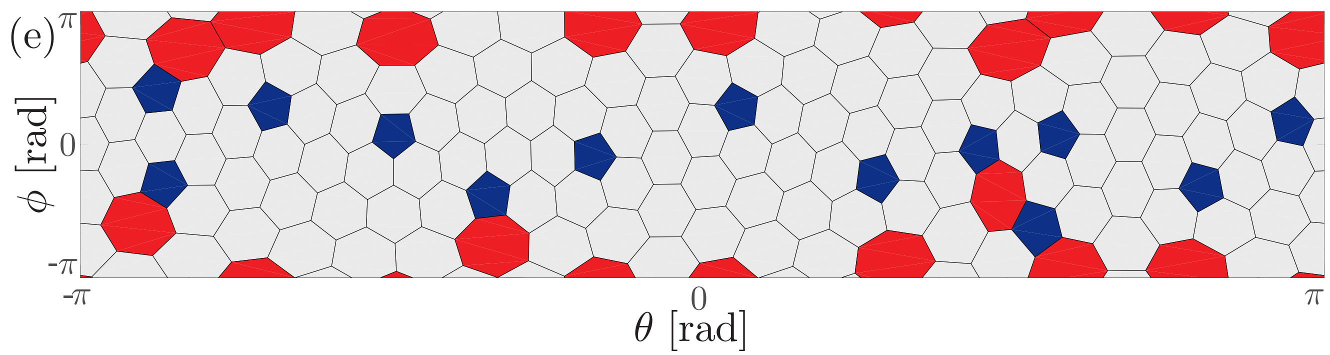
$$u_t = \gamma_0 \triangle u - \gamma_2 \triangle^2 u - au - bu^2 - cu^3 + \frac{h}{2}\left\{(\nu - 1)\left[b^{\alpha\beta}\nabla_\alpha u \nabla_\beta u + 2u\nabla_\beta\left(b^{\alpha\beta}\nabla_\alpha u\right)\right] + 2\nu\left[\mathcal{H}(\nabla u)^2 - 2\nabla\cdot(\mathcal{H}u\nabla u)\right]\right\} + \ldots$$

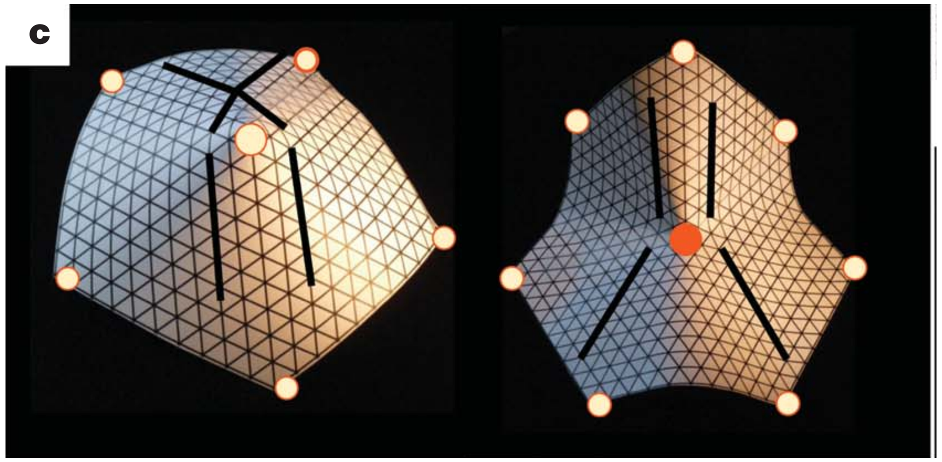


- $\mathcal{H} = b_\alpha^\alpha$: mean curvature
- Symmetry-breaking term could be "guessed"…!
- Curvature tensor non-constant on torus -> mixed phases possible
- Rubber (v=0.5): pure hexagonal phases for thin tori
  => restrict r/R=0.2

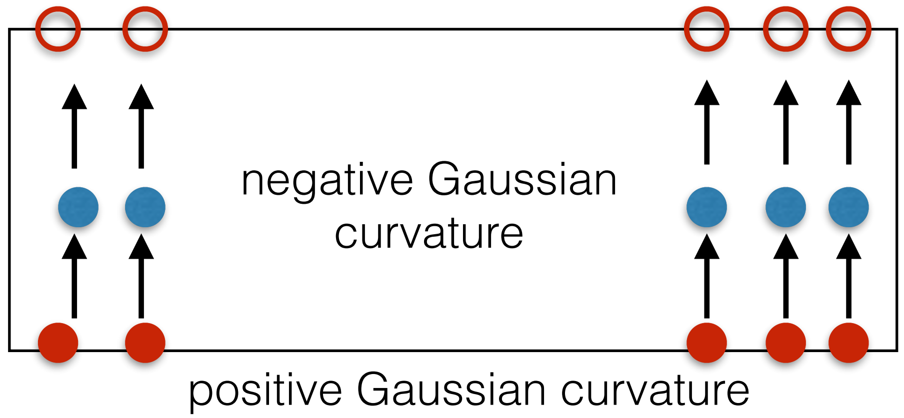
Defects on the torus

- Charge separation due to Gaussian curvature



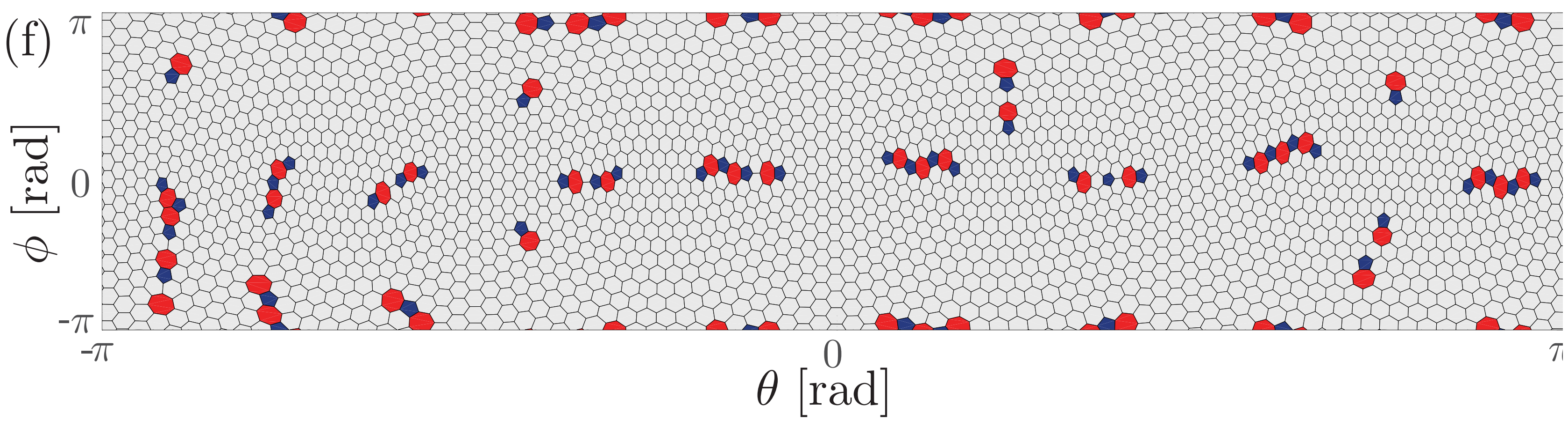


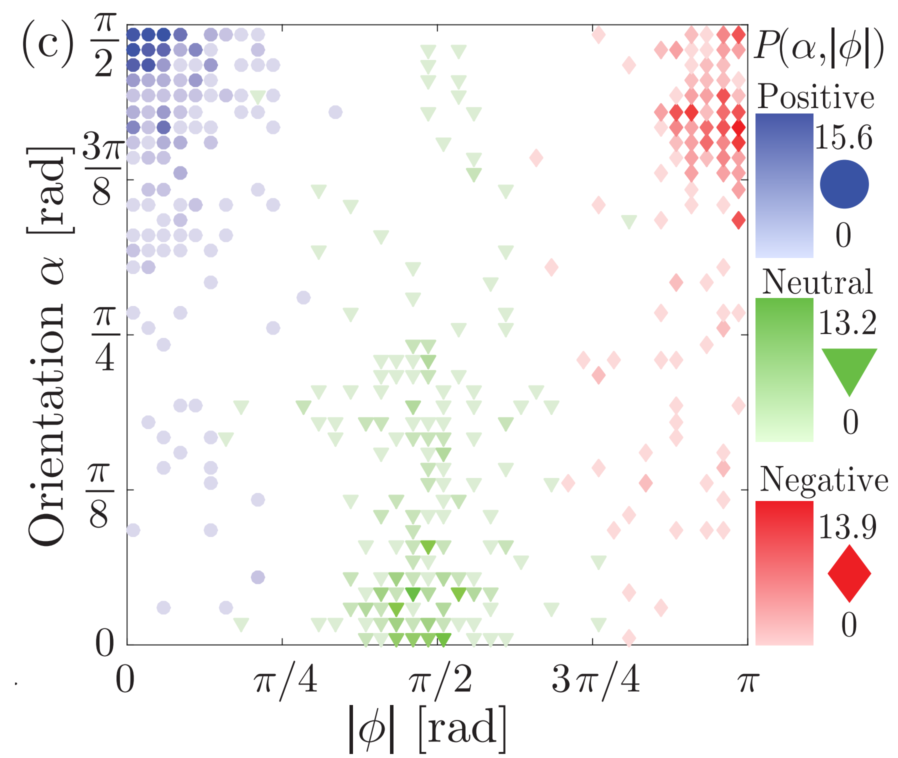
- Electrostatic analogy (M. Bowick et al, Phys. Rev. E 69, 2004)



Defects on the torus

- For larger system size, scars orient in this field





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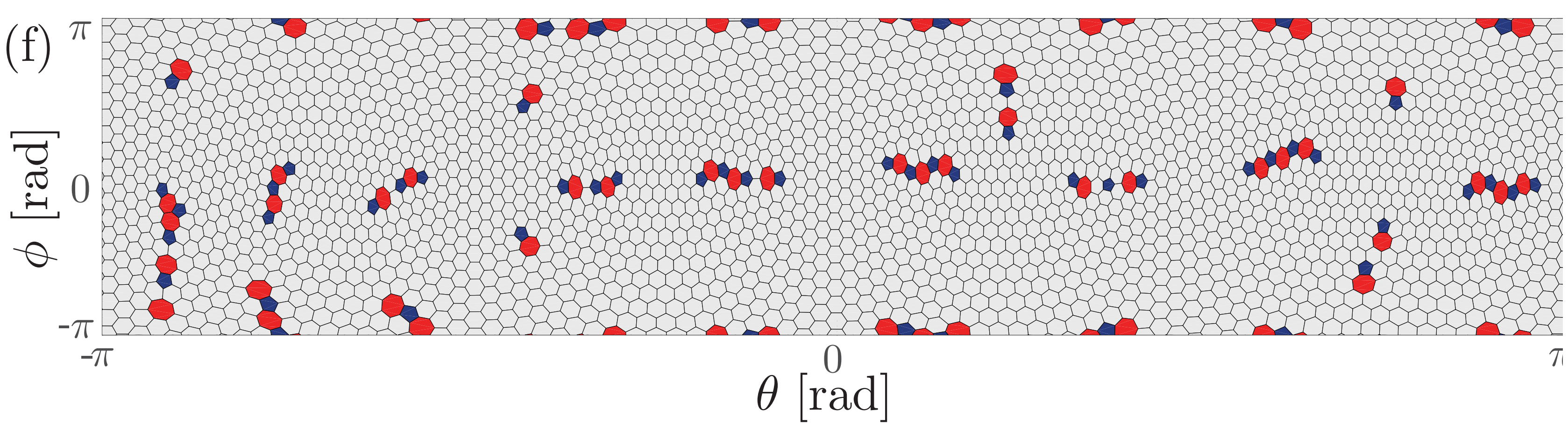

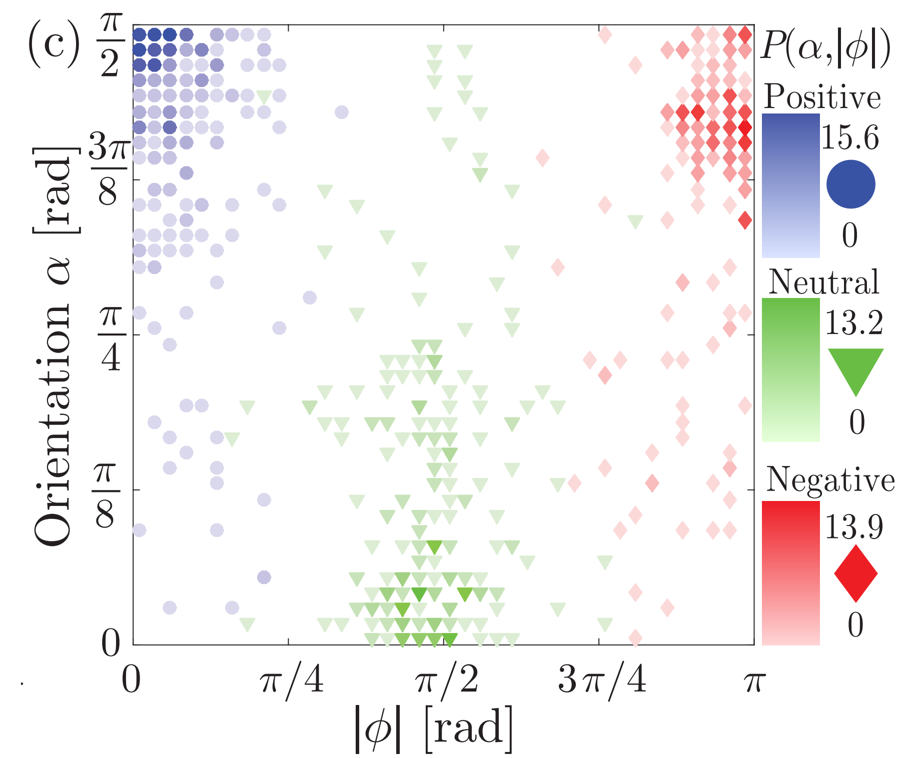

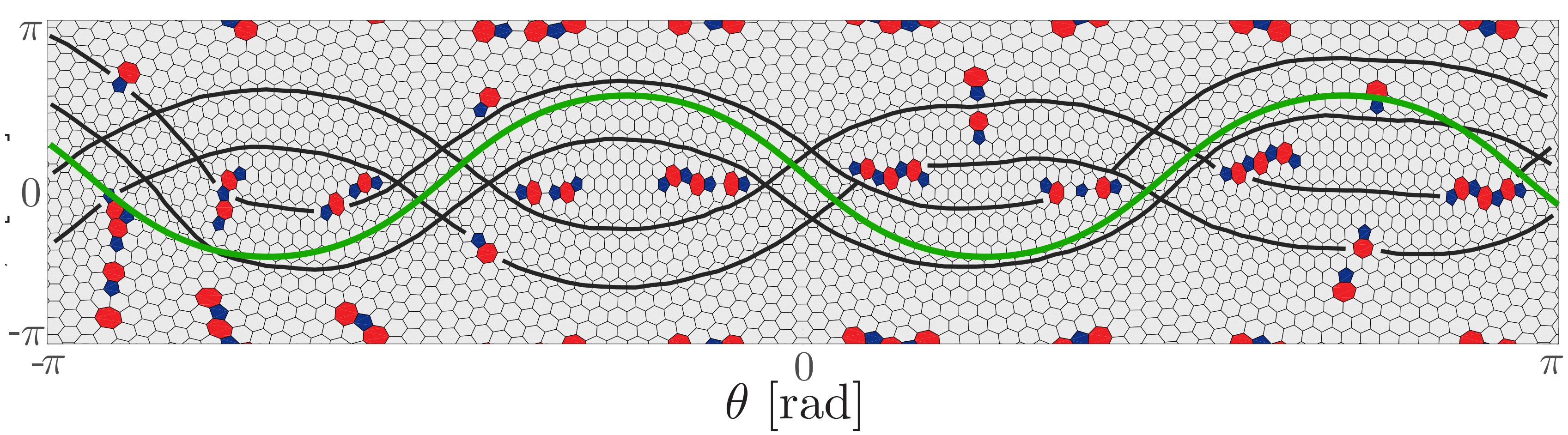

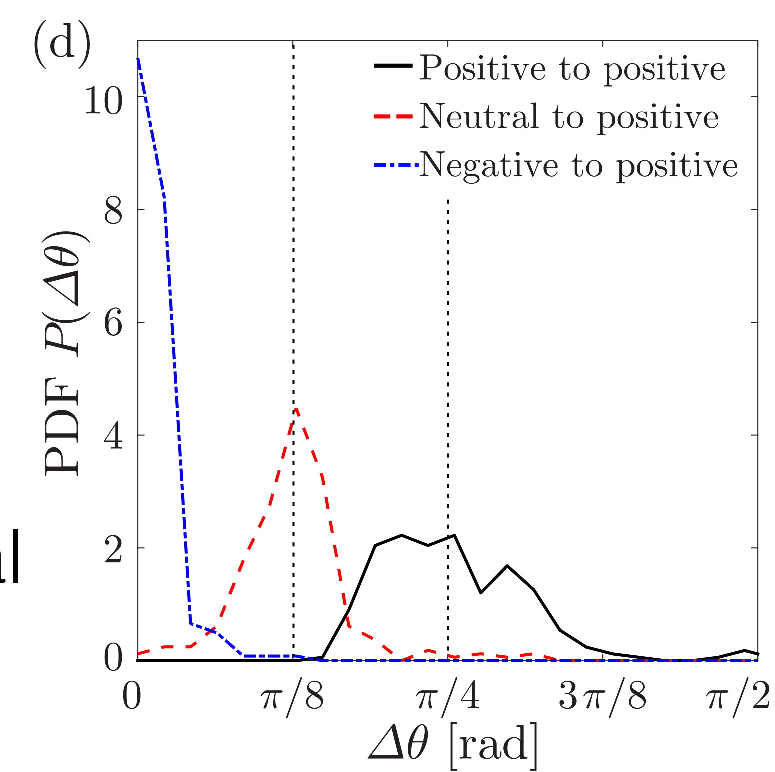

- Defects arranging along a geodesics with minimal total squared Gaussian curvature?

Conclusions

- Starting from the classical Koiter shell model, we systematically derived an effective wrinkling equation
- Matched to experiments, the theory reproduces qualitatively and quantitatively the morphologies and phase diagram of curved bilayer wrinkles.
- Wrinkling can be used to study defect formation on spheres and tori, with the later showing a “toroidal” superstructure.

Collaborators:

- Jörn Dunkel, Romain Lagrange, Francisco Jimenez, Pedro Reis, MIT
- Denis Terwange, ULB Bruxelles, Belgium

References:

- N. Stoop, R. Lagrange, D. Terwange, P. Reis, J. Dunkel, Curvature-induced symmetry-breaking determines elastic surface patterns, Nat. Mater. (2015)
- F. L. Jimenez, N. Stoop, R. Lagrange, J. Dunkel, P. Reis, Curvature-controlled defect localization in crystalline wrinkle patterns, arxiv.org/abs/1509.06547