Modeling Dynamics of Shape Transformation in “Blueprinted” Liquid Crystal Elastomers

Robin Selinger

Liquid Crystal Institute

Kent State University

Kent State will host International Liquid Crystal Conference
ILCC 2016

*** Abstracts due Feb 29 ***

Liquid Crystal Elastomer: Actuation mechanisms

First synthesized by Finkelmann group in 1991

R. Verduzco
Rice Univ.

Temperature

B. Ratna and
J. Naciri
Naval Research
Laboratory

Electric Field

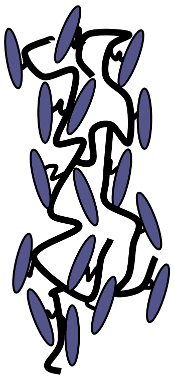
C. Spillman, J. Naciri, and
B. Ratna
Naval Research Laboratory

Photoexcitation

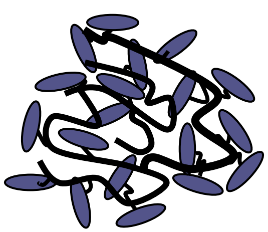
TJ White et al
AFRL

Actuation mechanisms

Nematic elastomer

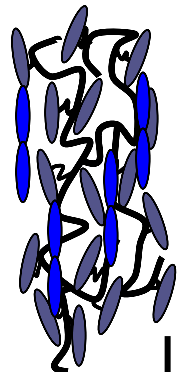


Raise Temperature

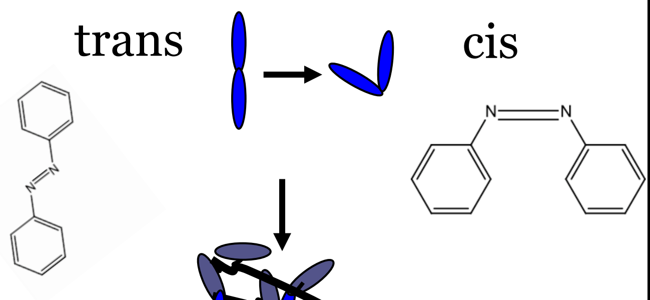


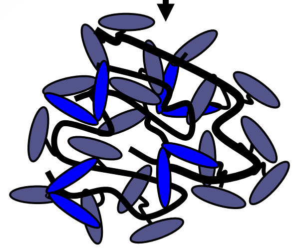
Isotropic

Nematic+azo dye



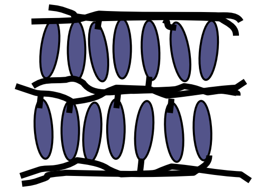
Photoexcitation



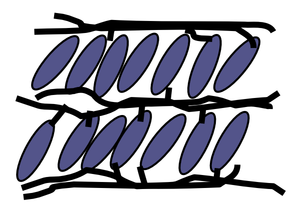


Disrupts order

Smectic elastomer



Electric field induces tilt

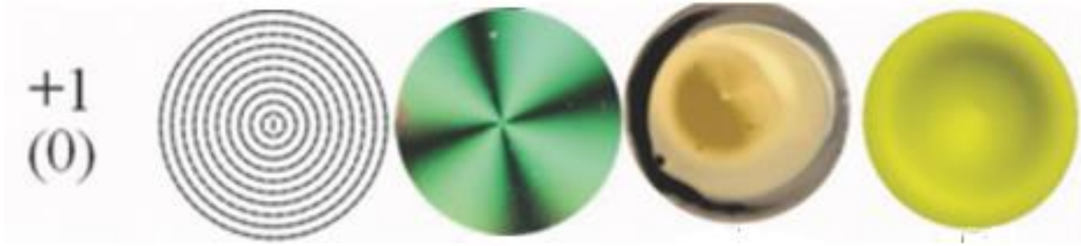


Layer contraction

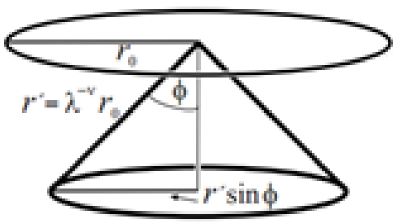
“Blueprinted” nematic LCE:
formed between patterned substrates

Non-uniform strain drives shape change, curvature, buckling...

Complete trajectory of motion encoded in director field



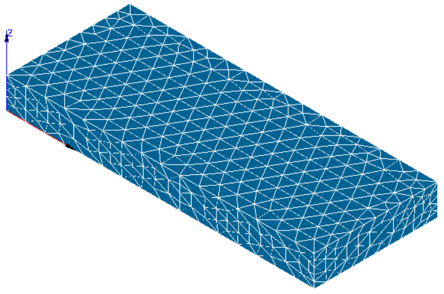
McConney et al
Advanced Matls 2013



Carl Modes et al
PRE 2010

De Haan et al
Angewandte Chemie 2012

Modeling shape change in elastic solids: finite element elastodynamics



Tetrahedral mesh:

Nodes at corners of volume elements

Hamiltonian approach to model elastic medium…

$$H = \sum_{elements\ n} \left[\frac{1}{2} C_{ijkl} \varepsilon_{ij}^{n} \varepsilon_{kl}^{n} \right] V_n + \sum_{nodes\ p} \left[\frac{1}{2} m_p v_p{}^2 \right]$$

Elastic potential energy
(Nonlinear: Green-Lagrange strain)

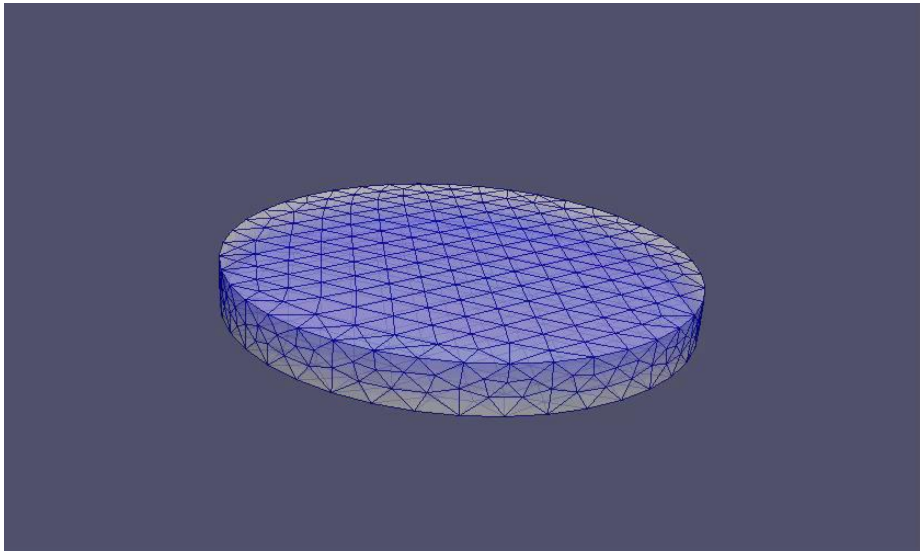
$U_{potential}$

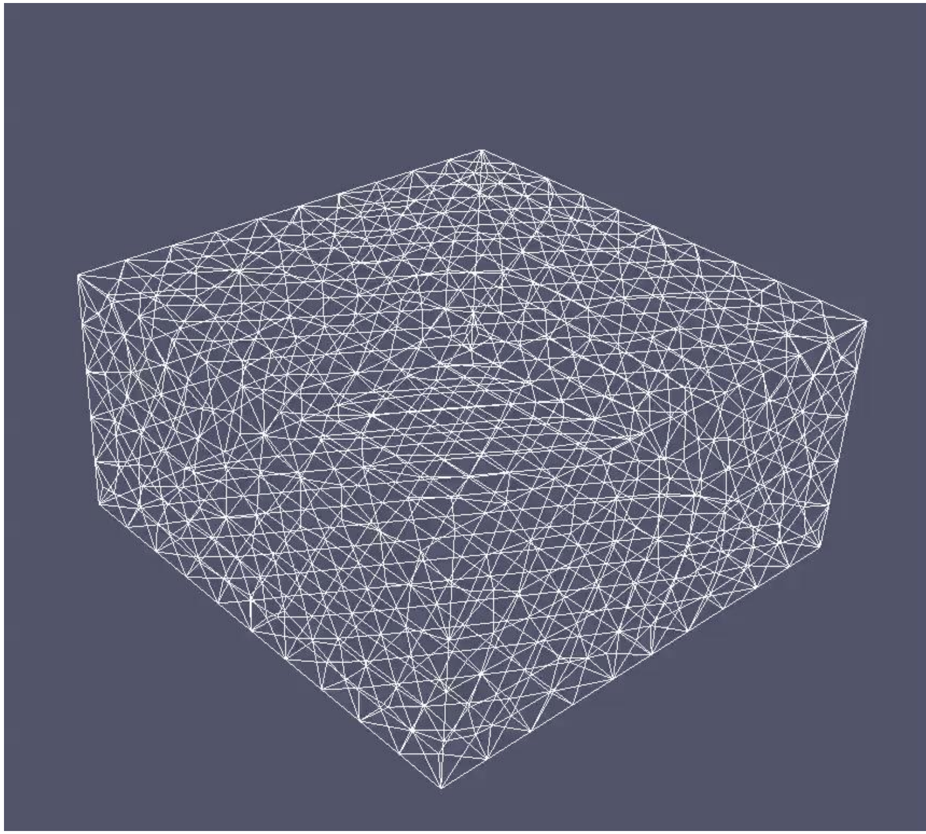
Kinetic energy
(lumped mass approximation)

Nodes move via $f = ma$ $$m\ddot{r}_n = -\frac{\partial U_{pot}}{\partial r_n}$$

Home-made code implemented in CUDA for GPU-enabled computer

Fast nonlinear 3-d elastodynamics

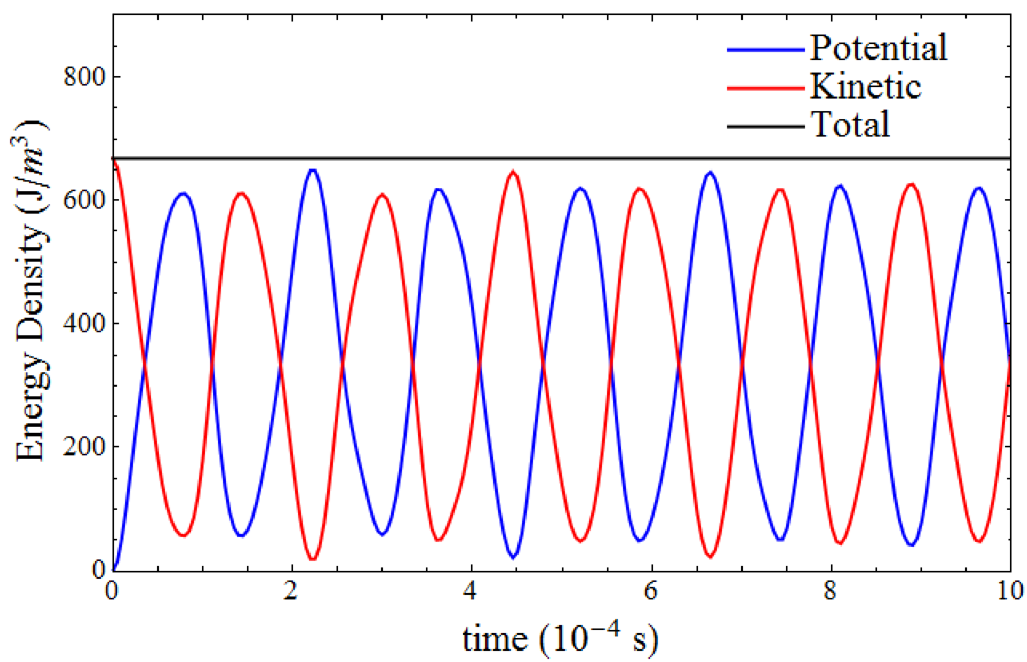




Code runs at 700 frames/second

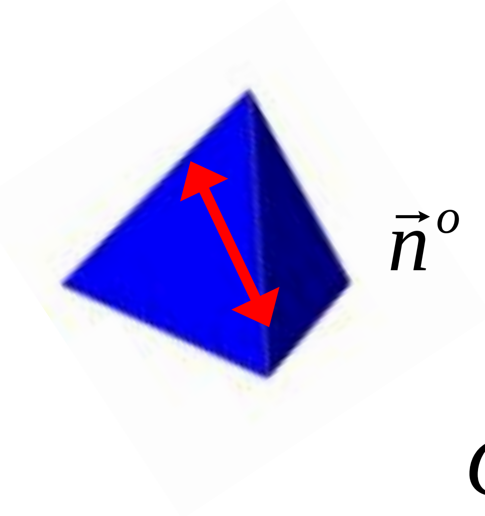
Without dissipative forces added, kinetic+potential energy is well conserved

Must add friction/dissipation to relax to mechanical equilibrium



Sum of kinetic+potential energy is constant

Modeling nematic elastomers…



$\vec{n}^{o}$ = blueprinted director

Use tensor form

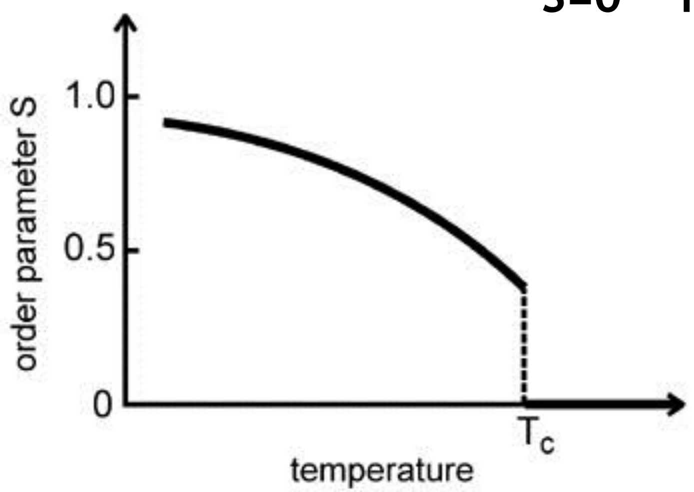
$$Q_{ij} = \frac{1}{2}\left(3n_i n_j - \delta_{ij}\right)$$

Q_{ij}^{0} → Describes nematic order at cross-linking defined in each volume element

$Q_{ij} = S(T)\,Q_{ij}^{0}$ → **S = scalar order parameter, drops on heating**

S=1 perfect nematic order

S=0 isotropic



Scalar order parameter drops with temperature

$$H = \sum_{elements\ n}\left[\frac{1}{2}C_{ijkl}\varepsilon_{ij}^{n}\varepsilon_{kl}^{n} - \alpha\left(Q_{ij} - Q_{ij}^{o}\right)_n \varepsilon_{ij}^{n}\right]V_n + \sum_{nodes\ p}\left[\frac{1}{2}m_p v_p^{\ 2}\right]$$

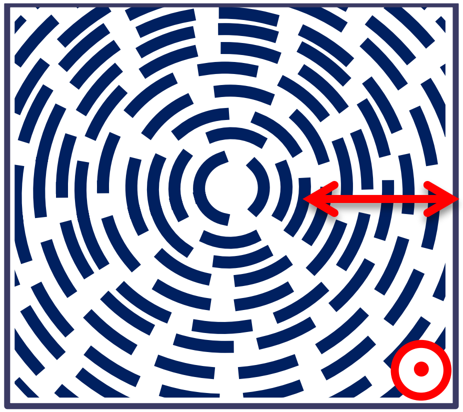
Elastic potential energy U_{pot}

Couples strain and nematic order

Kinetic energy

Q_{ij} changes with temperature (or other stimulus)

Changing Q_{ij} changes the local metric → shape change

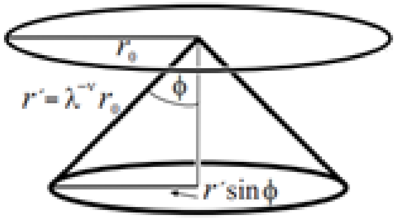


Modes and Warner predicted:

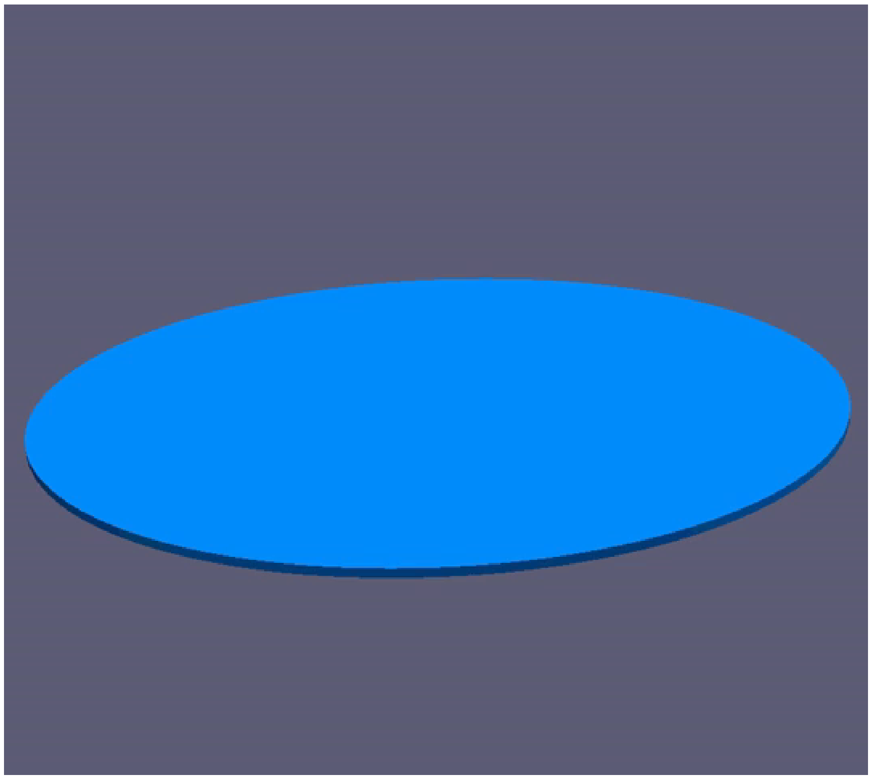
C. D. Modes et al, *PRE* 2010

$T > T_{flat}$ (high T range)

Cone



Azimuthal +1
blueprinted director field:



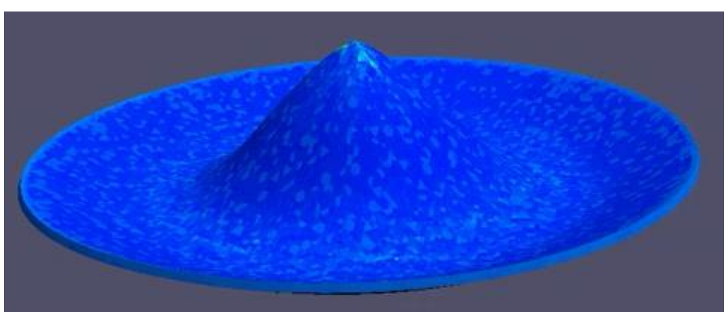
Includes bending energy:

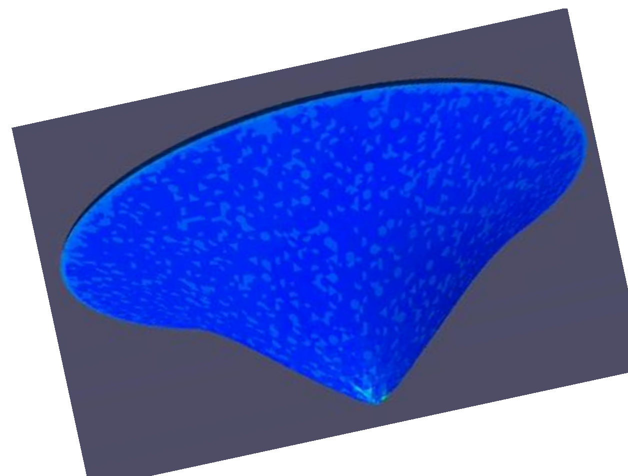
“sombrero” snaps through to cone

Compare with experiments….

McConney et al
Advanced Materials, 2013

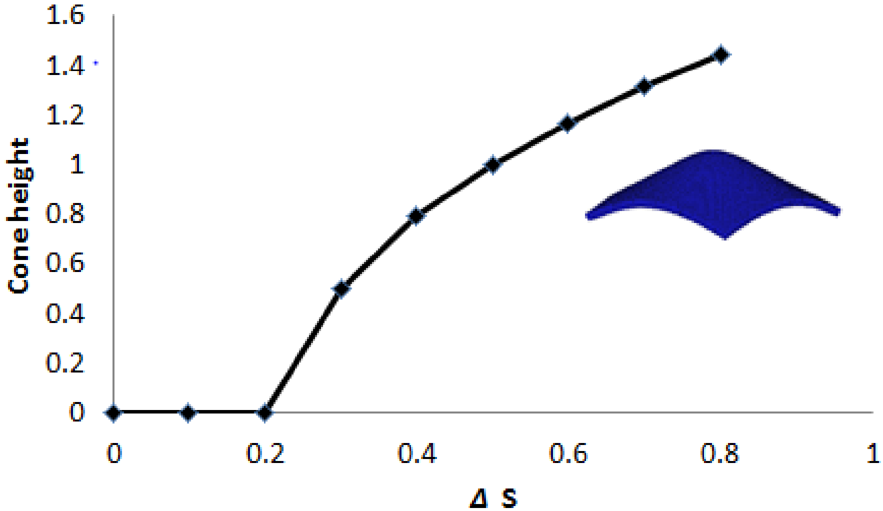
De Haan, et al.
Angewandte Chemie 2012





+1 defect

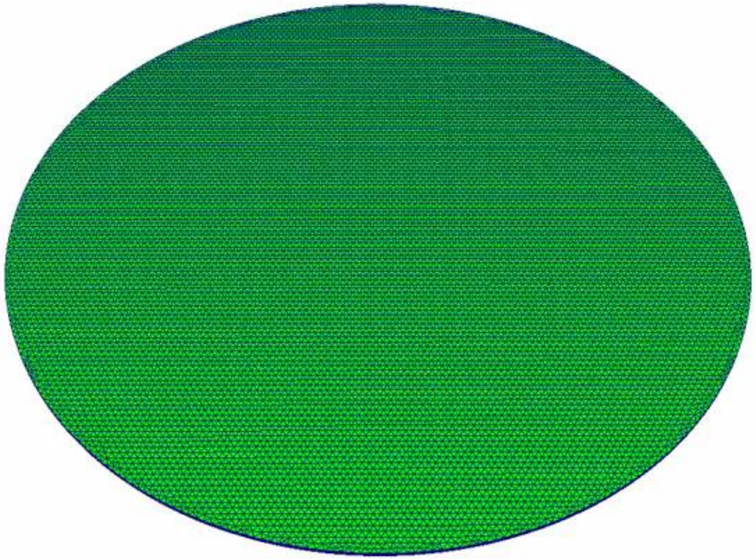
-1 defect



Cone height as a function of ΔS

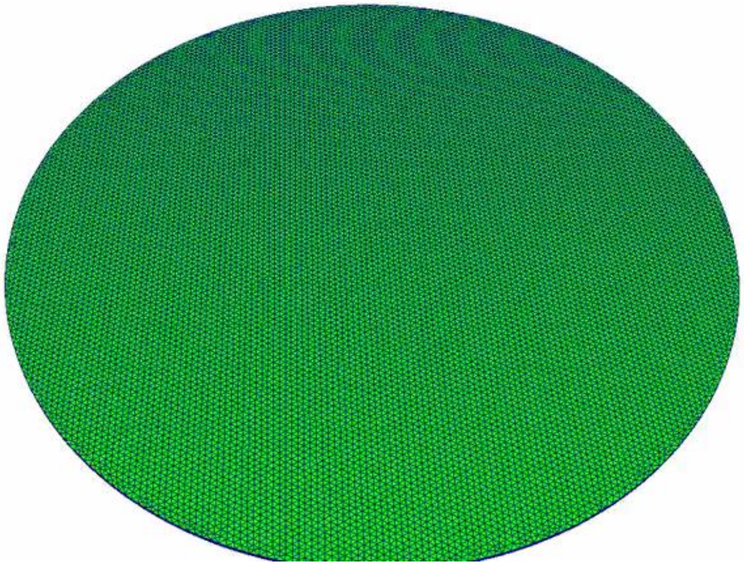
cone emerges only when heated sufficiently that $\Delta S \geq 0.3$

Sample aspect ratio 50:1



Heat uniformly…
Up-down symmetry→ metastable state

-4 defect



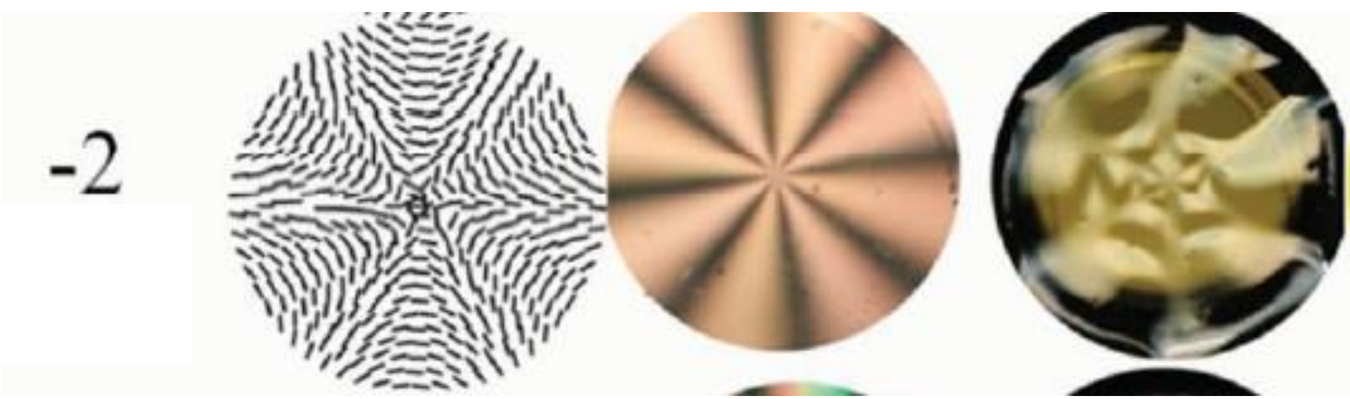
Heat from one side→breaks symmetry

Negative defects:

-2 defect, heating

Color=strain energy density

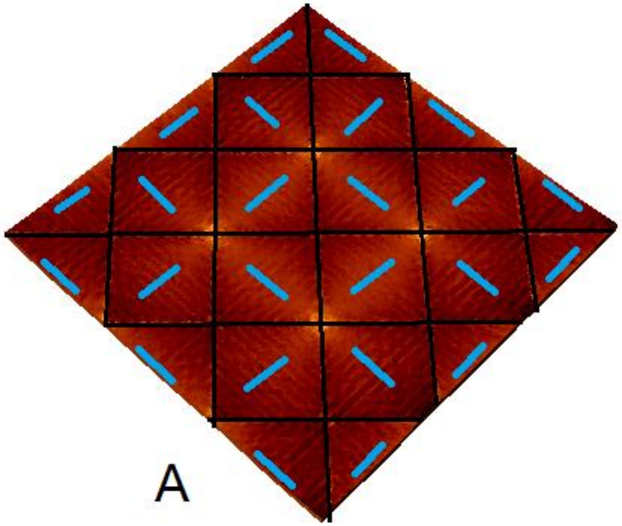
Residual strain present in transformed state



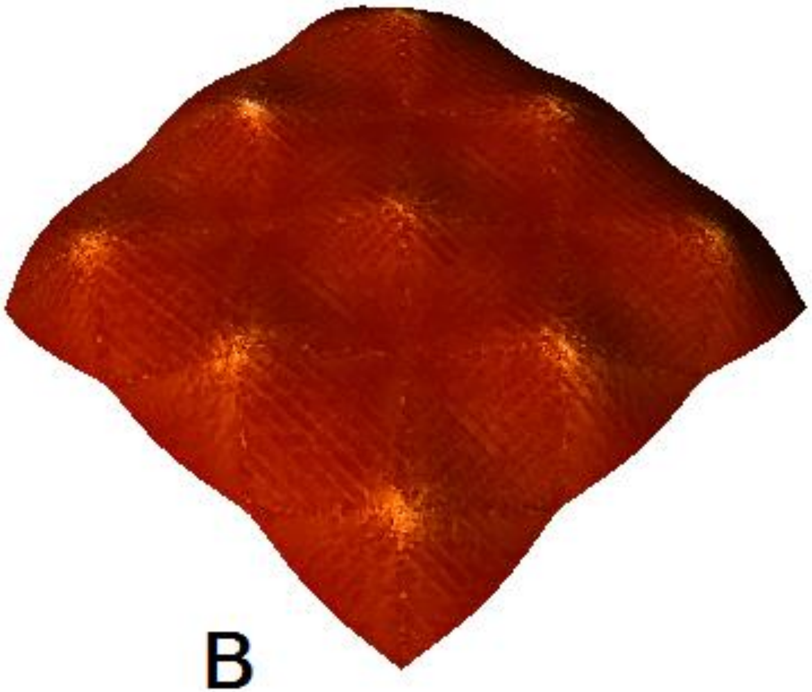
McConney et al
Advanced Materials 2013

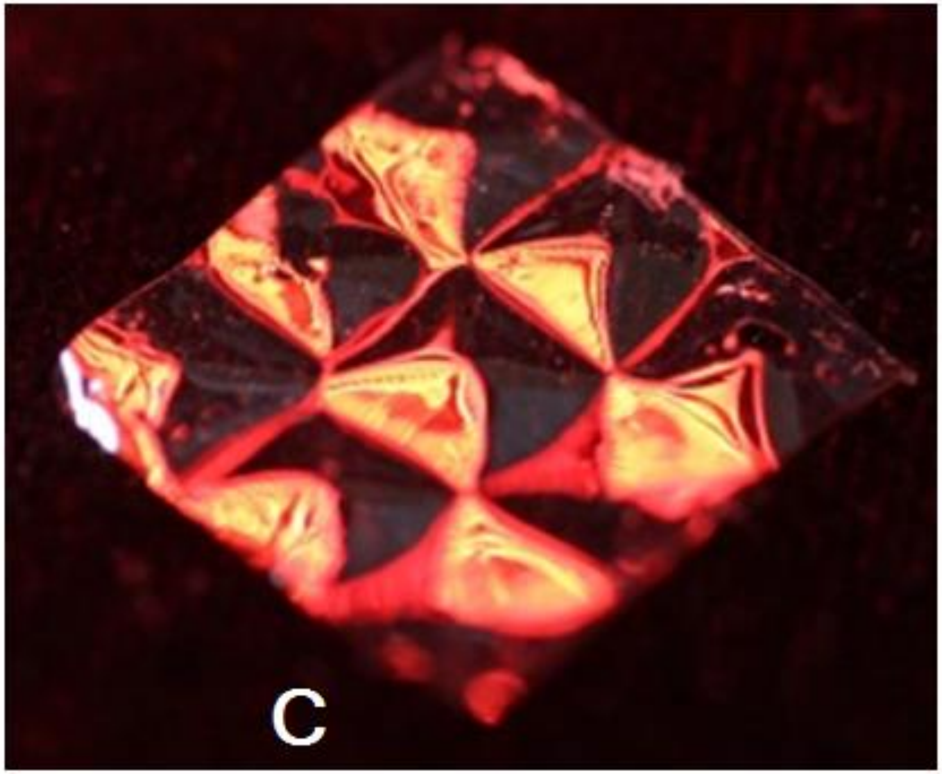
Compare w/ experiments
by McConney and White, AFRL

Blueprinted
director field

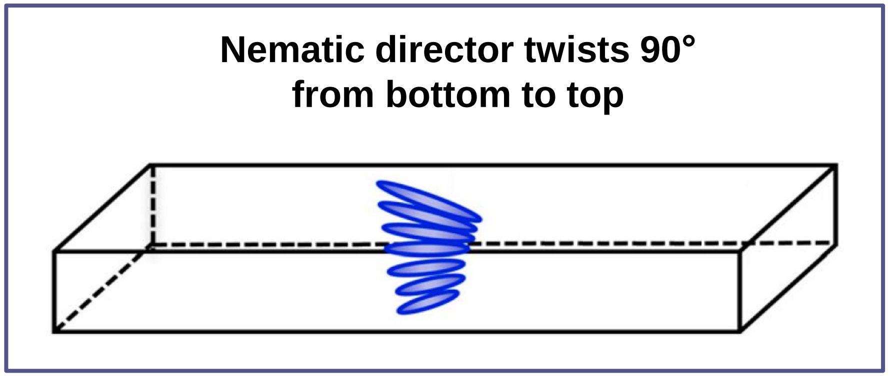


Finite Element
simulation

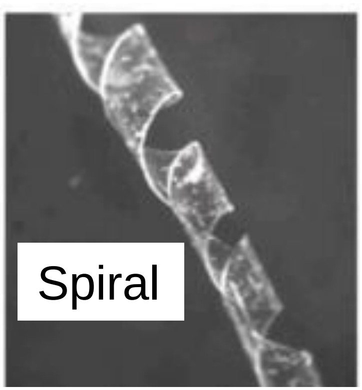




Experiments by Kenji Urayama: Twisted nematic elastomer ribbons



$\vec{n}$

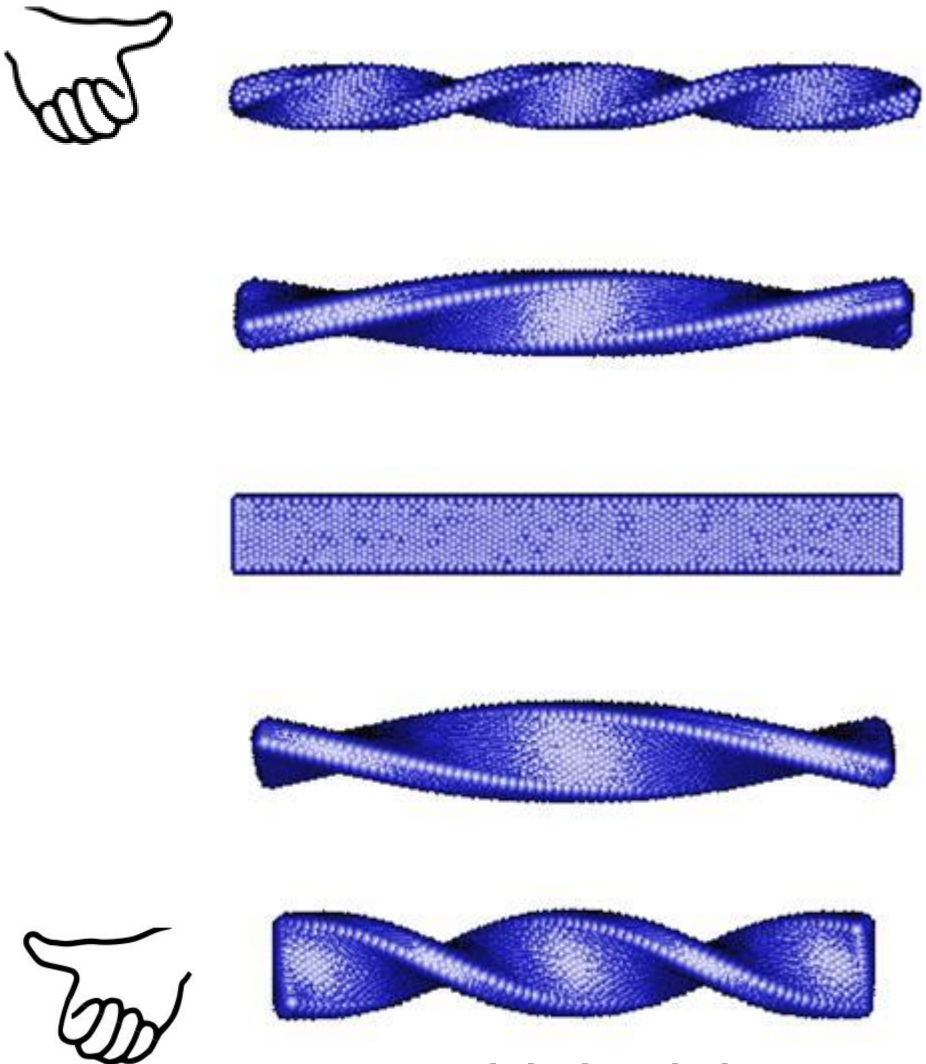


Y. Sawa, F. Ye, K. Urayama, T. Takigawa, V. Gimenez-Pinto, R. L. B. Selinger, J. V. Selinger ***PNAS* 2011**

Chirality reversal with temperature

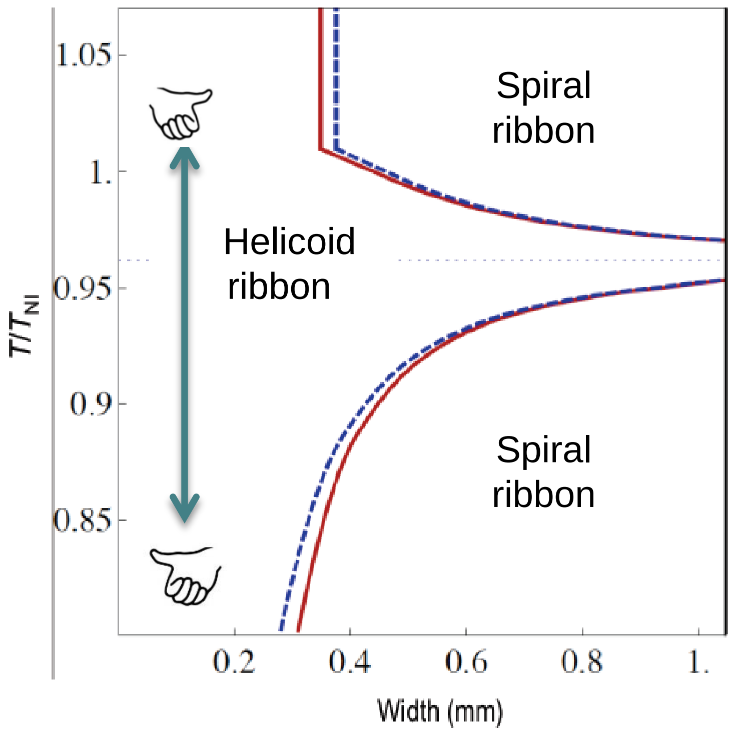
FEM simulation, aspect ratio 50-5-1

High T : Left-handed



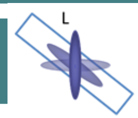
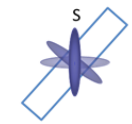
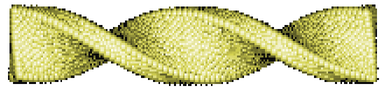
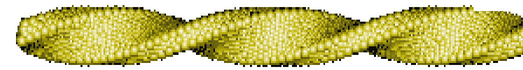
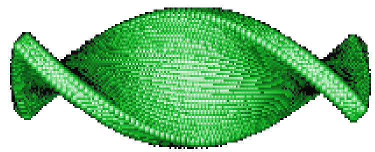
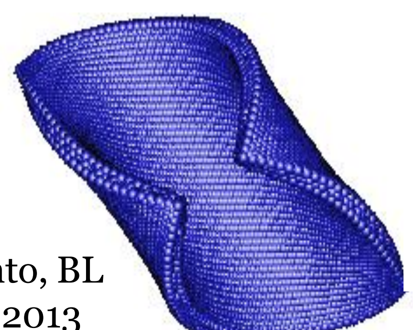
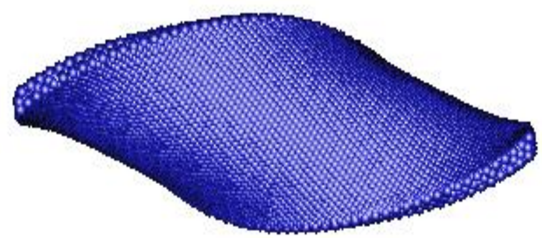
Low T : Right-handed

Theoretical predicted phase diagram



Y. Sawa, F. Ye, K. Urayama, T. Takigawa, **V. Gimenez-Pinto**, R. L. B. Selinger, J. V. Selinger ***PNAS* 2011**

Helicoid or Spiral? Shape depends on twist geometry. aspect ratio

Aspect ratio	Equilibrium shape	L geometry 	S geometry 
50-5-1	Helicoid ribbon		
50-10-1	Helicoid ribbon		
50-15-1	Helicoid ribbon		
50-20-1	Helicoid ribbon		
50-25-1	Spiral ribbon		

Pitch grows

Shape transition

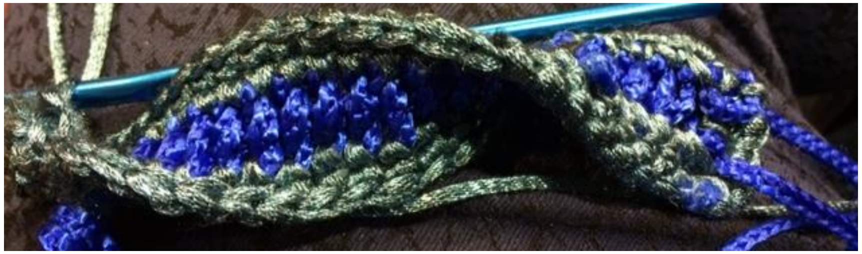
Y Sawa, KUrayama, T Takigawa, V Gimenez-Pinto, BL Mbanga, F Ye, JV Selinger, RLBS, Phys. Rev. E 2013

Just for fun… the fiber arts version

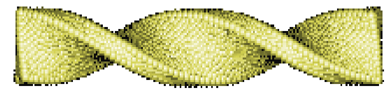
Start with chiral helicoid
(made with handed knots: **Macramé**)

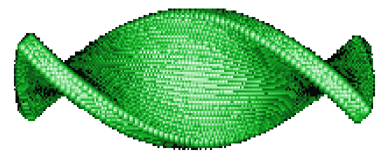
Use crochet to add width…

Observe resulting shape changes



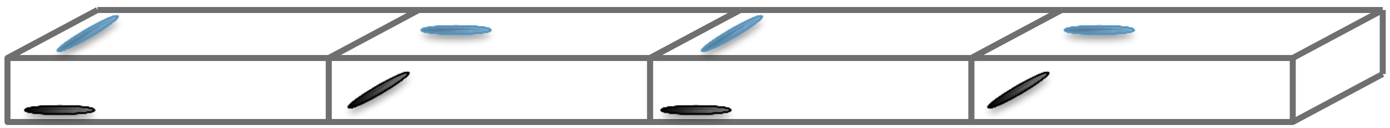
Just for fun... the fiber arts version

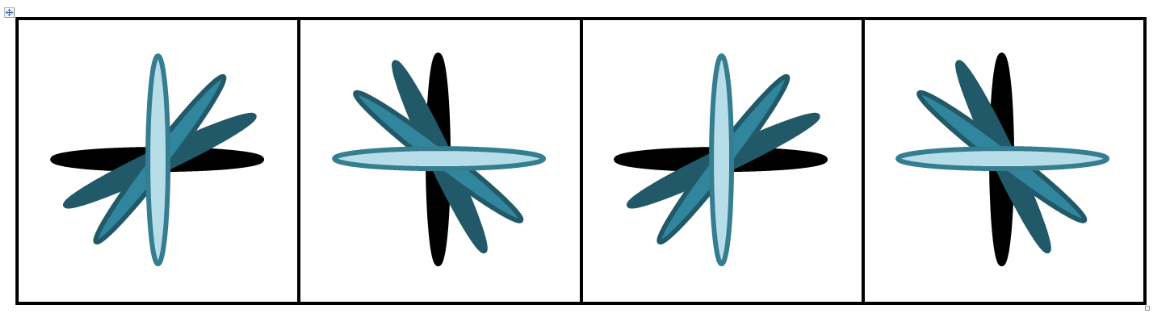




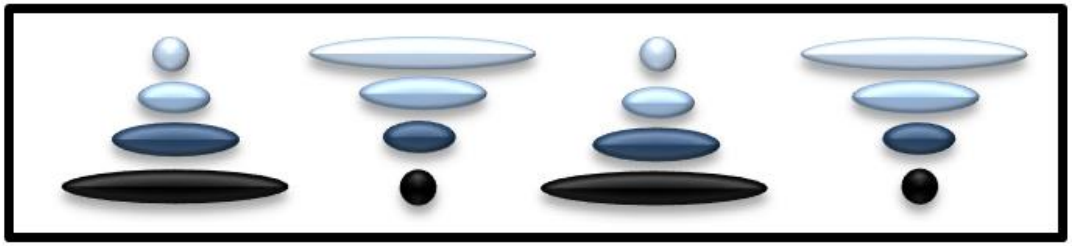
More complex microstructures: twisted domains

Thin sample with alternating twisted domains





Top view

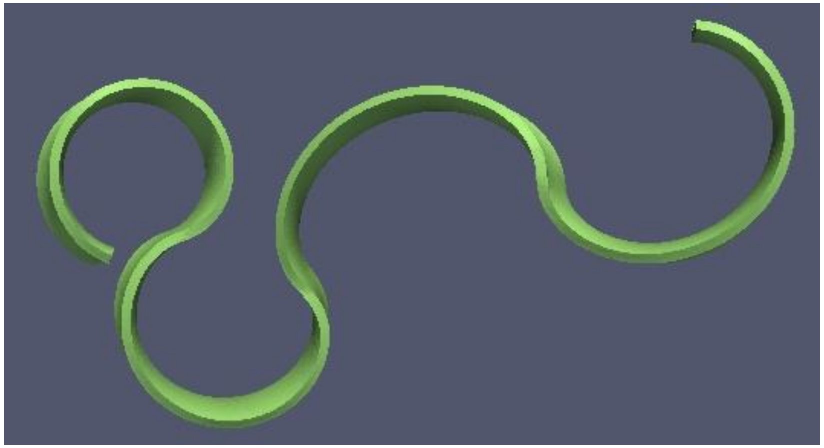


Side view

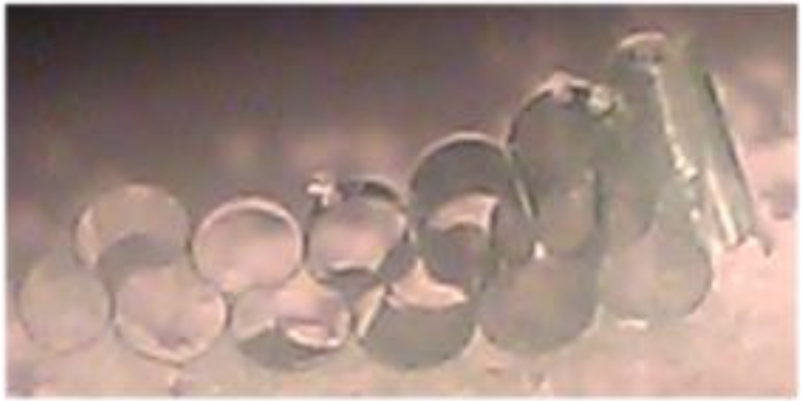
Teardrop folds

When stripe width/thickness is large enough ($s_w/t \geq 200$)
Sample forms "Teardrop" folds

FEM simulations

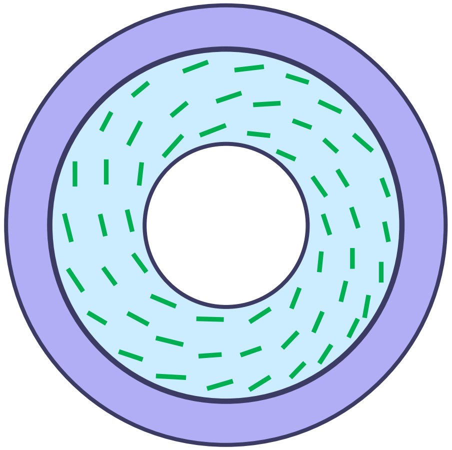


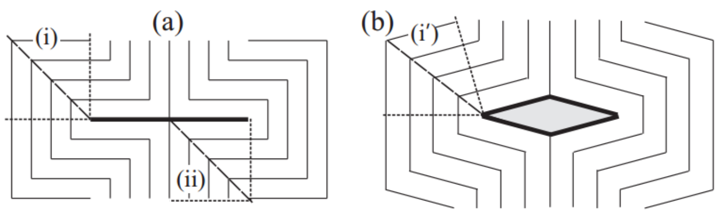
Experiments by De Haan et al.
Eindhoven group



LT de Haan, V Gimenez-Pinto, A Konya,
TS Nguyen, JMN Verjans,
C Sánchez-Somolinos, JV Selinger,
RLB Selinger, Dirk Broer, APHJ Schenning
Advanced Functional Materials 2014

Blueprinted chiral iris
with shallow grooves



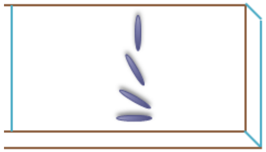


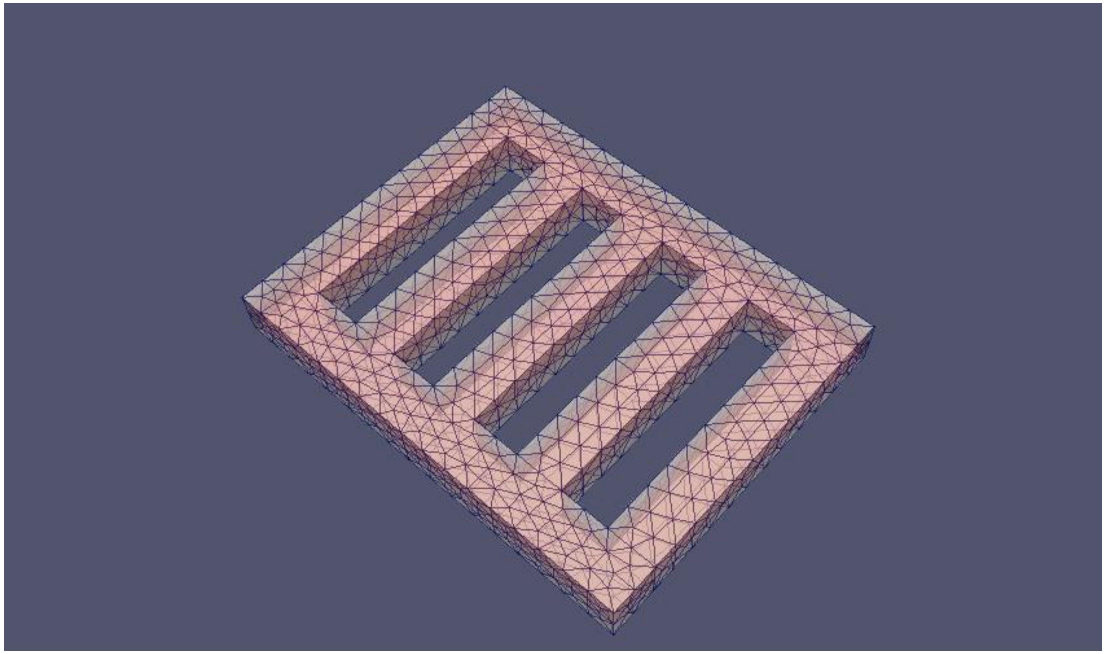
cold hot

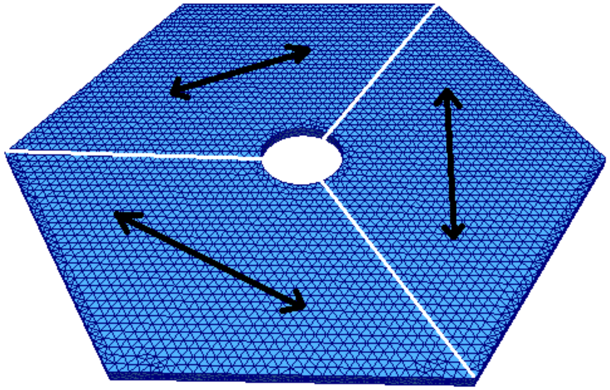
Angular Deficits in Flat Space: Remotely Controllable Apertures in Nematic Solid Sheets ***C.D. Modes, M. Warner, C. Sanchez-Somolinos, L.T. de Haan, D. Broer***
Proc. R. Soc. A, 2012

Designer shapes assembled from simple motifs

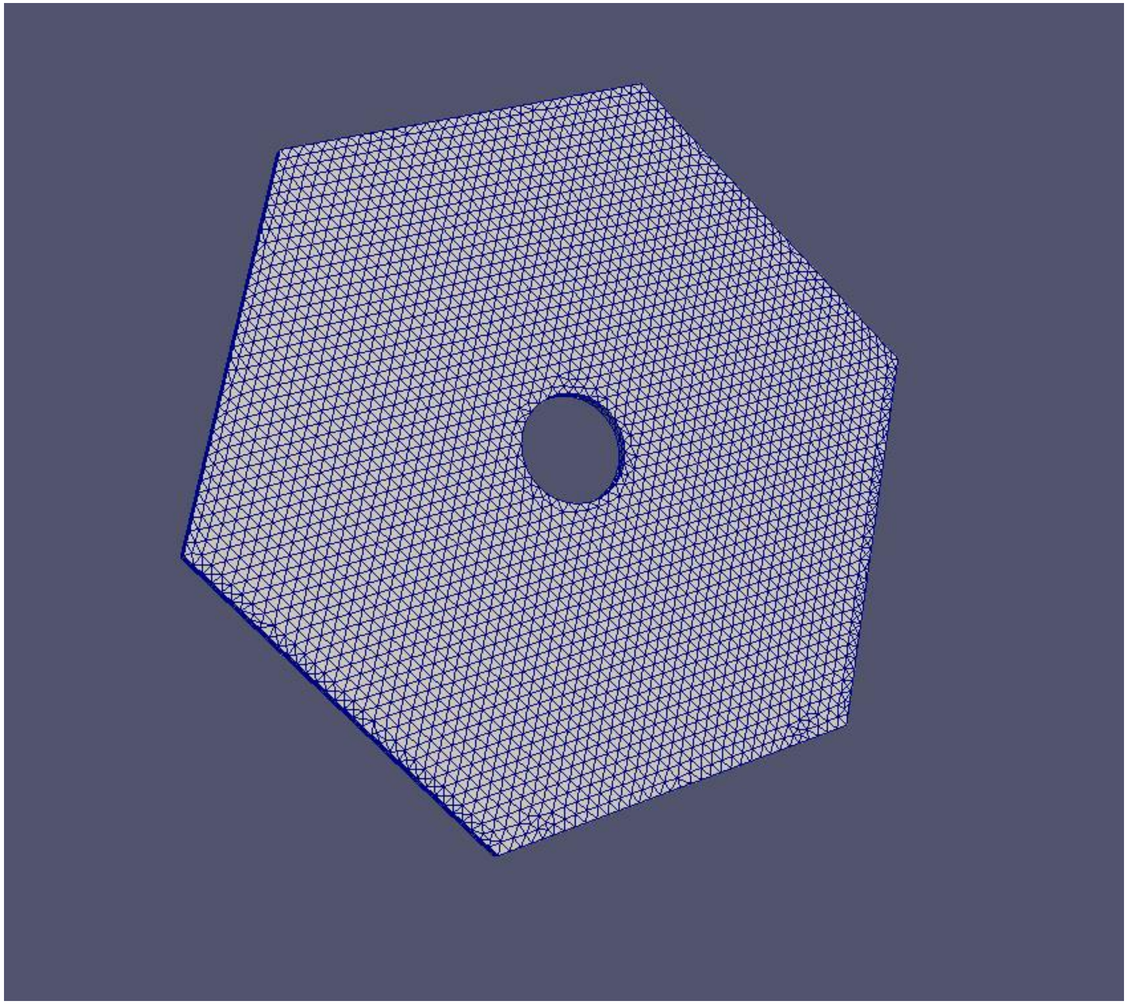
Splay hinge with cut-outs to accommodate transverse strain

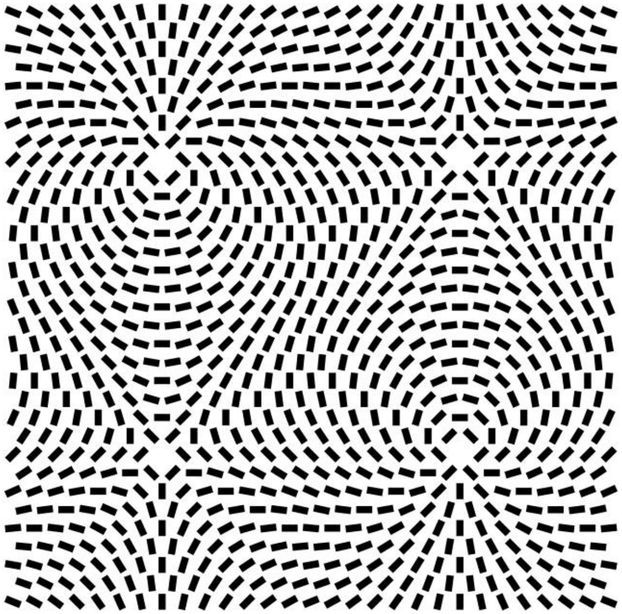






Making a corner:
Director pattern proposed by Carl Modes
Tip cut out to avoid stress divergence



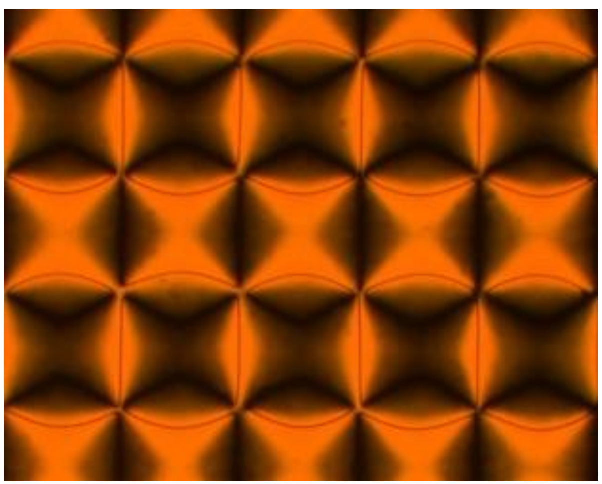


Blueprinting complex director structures

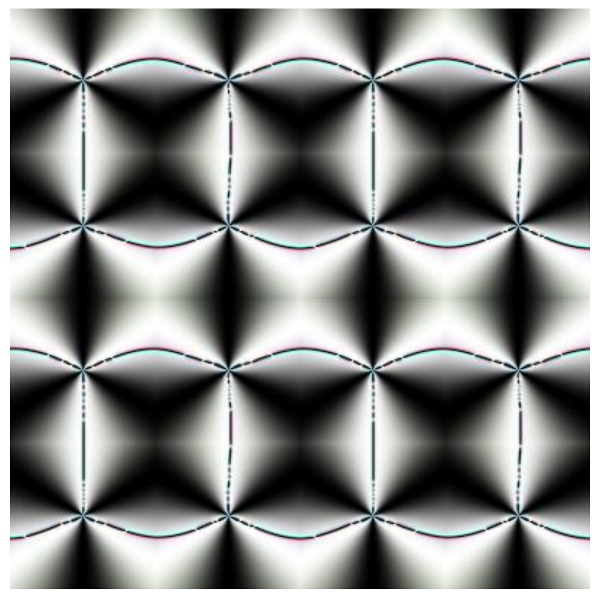
+ / - (3/2) defect array on one surface

Planar on the other surface ←→

Minimize Frank energy in 3D to find microstructure…



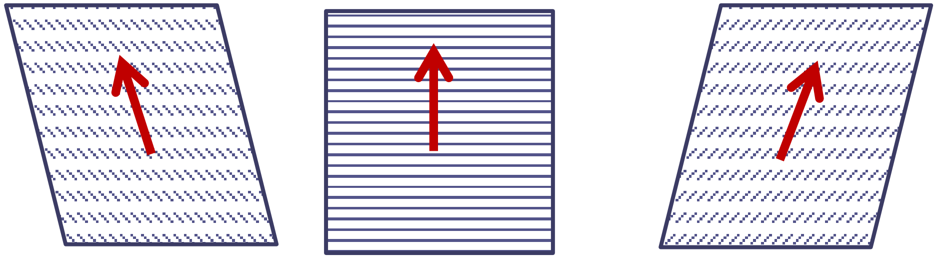
Experiment – Qihuo Wei



Simulation

Coming soon:
Crosslink
to form
LC elastomer

Smectic film actuated with alternating electric field
Electroclinic effect: Director tilts left/right

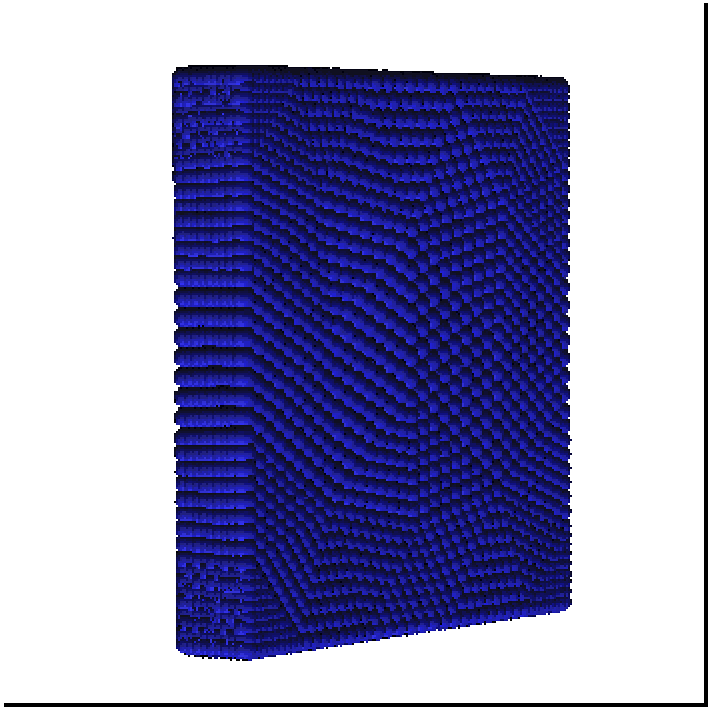


Expect shear deformation…

But it twists instead

Smectic film actuated with alternating electric field
Electroclinic effect: Director tilts left/right (like a metronome)

Front/back asymmetry: gradient in strain-order coupling induces twist

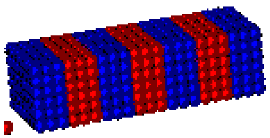


Modeling self-propelled robots

Modulate nematic order parameter in a wave pattern

Choose wavelength such that head and tail are out of phase

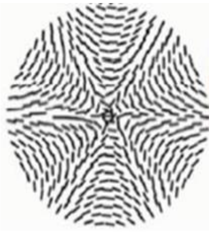
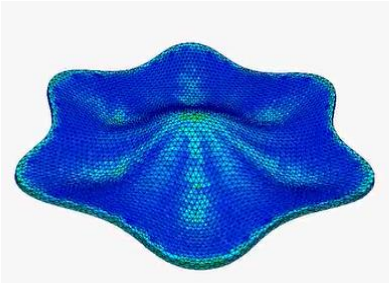
Assume perfect one-way static friction



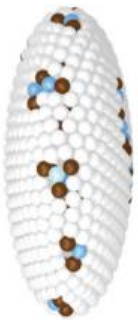
$$Q_{ij} = q\, e^{\mathbf{i(kx\text{-}wt)}} \begin{bmatrix} 1 & 0 & 0 \\ 0 & -0.5 & 0 \\ 0 & 0 & -0.5 \end{bmatrix}$$

The BIG Picture…

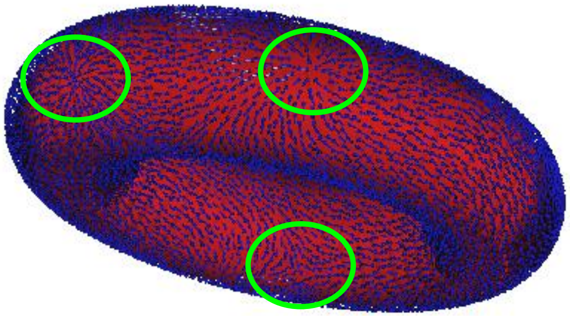
1. Microstructure is fixed but shape changes:
- Blueprinted LC Elastomer

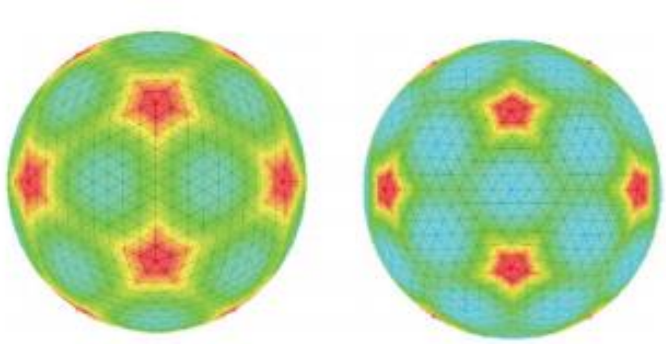
2. Shape is fixed but microstructure changes:
- Orientational ordered thin film on a curved surface
- Crystalline solids on a curved surface
- See review by Bowick and Giomi, *Advances in Physics 2009*



Burke et al
Soft Matter 2015



RLBS, A Konya, Al, and JV Selinger
J. Phys. Chem. B, **2011**

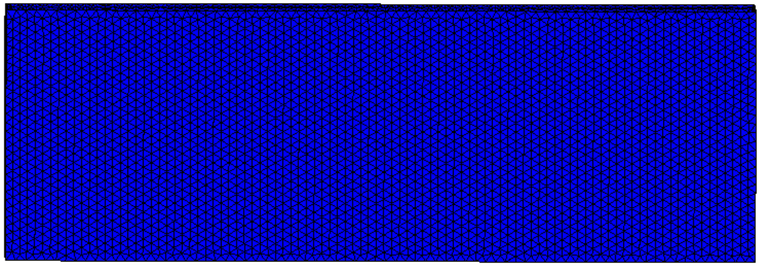


MJ Bowick and L Giomi,
Advances in Physics 2009

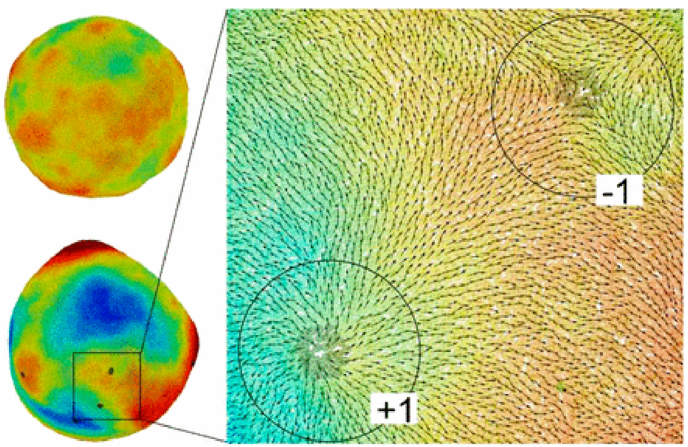
More challenging case: Both shape and microstructure change

- Soft elastic response in LC elastomers

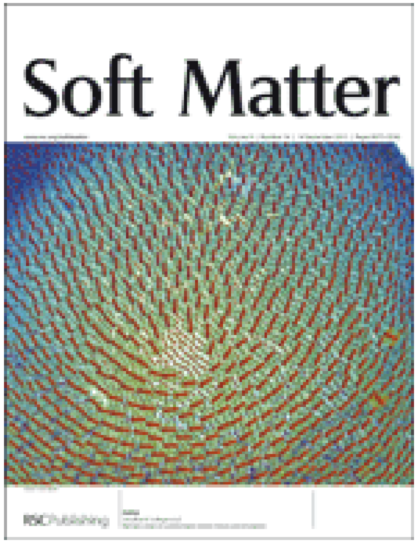
  M. Mbanga, F. Ye, J. Selinger, RLBS
  PRE 82, 051701 (2010)



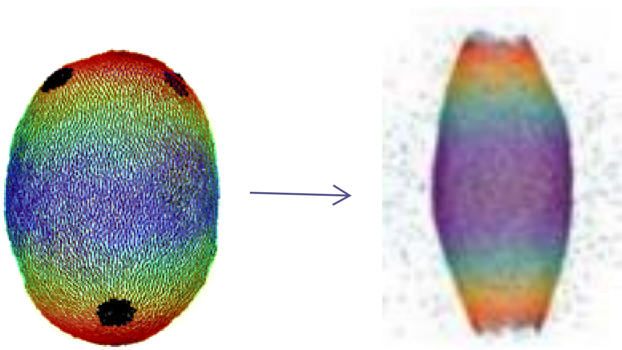
- Lipid membranes with in-plane orientational order



LS Hirst, A Ossowski, M Fraser, J Geng, JV Selinger, and RLBS
PNAS 2013

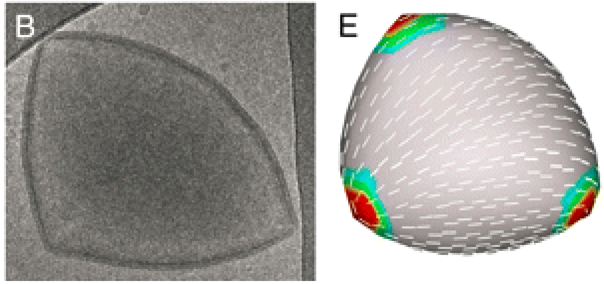


TS Nguyen, J Geng, RLBS, JV Selinger
Soft Matter 2013

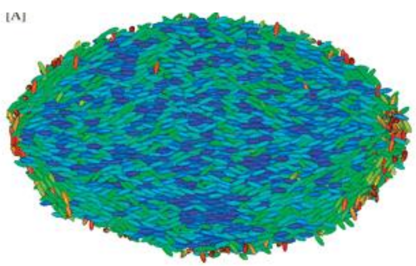


Morphology change

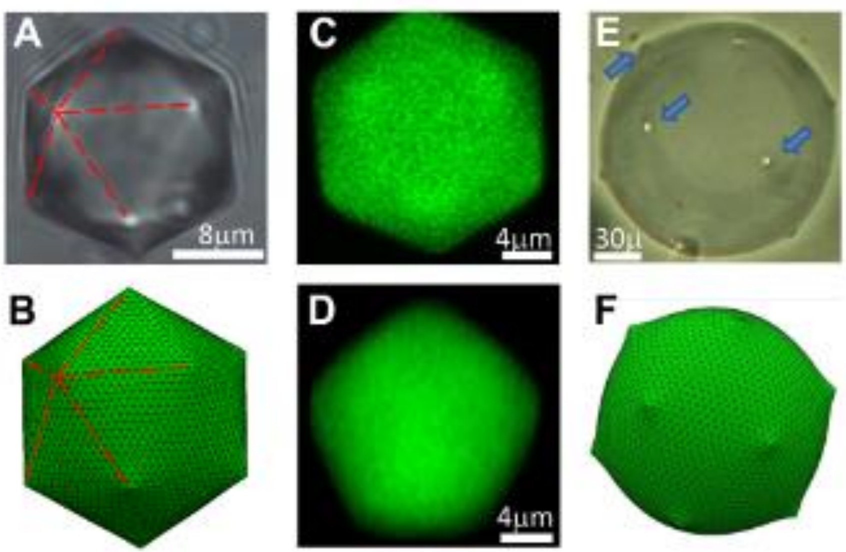
Kinetic competition between defect motion and shape evolution can produce defect-rich metastable states



Morphology of nematic and smectic vesicles
X Xing, H Shin, M Bowick, Z Yao, L Jia, MH Lui
PNAS 2012



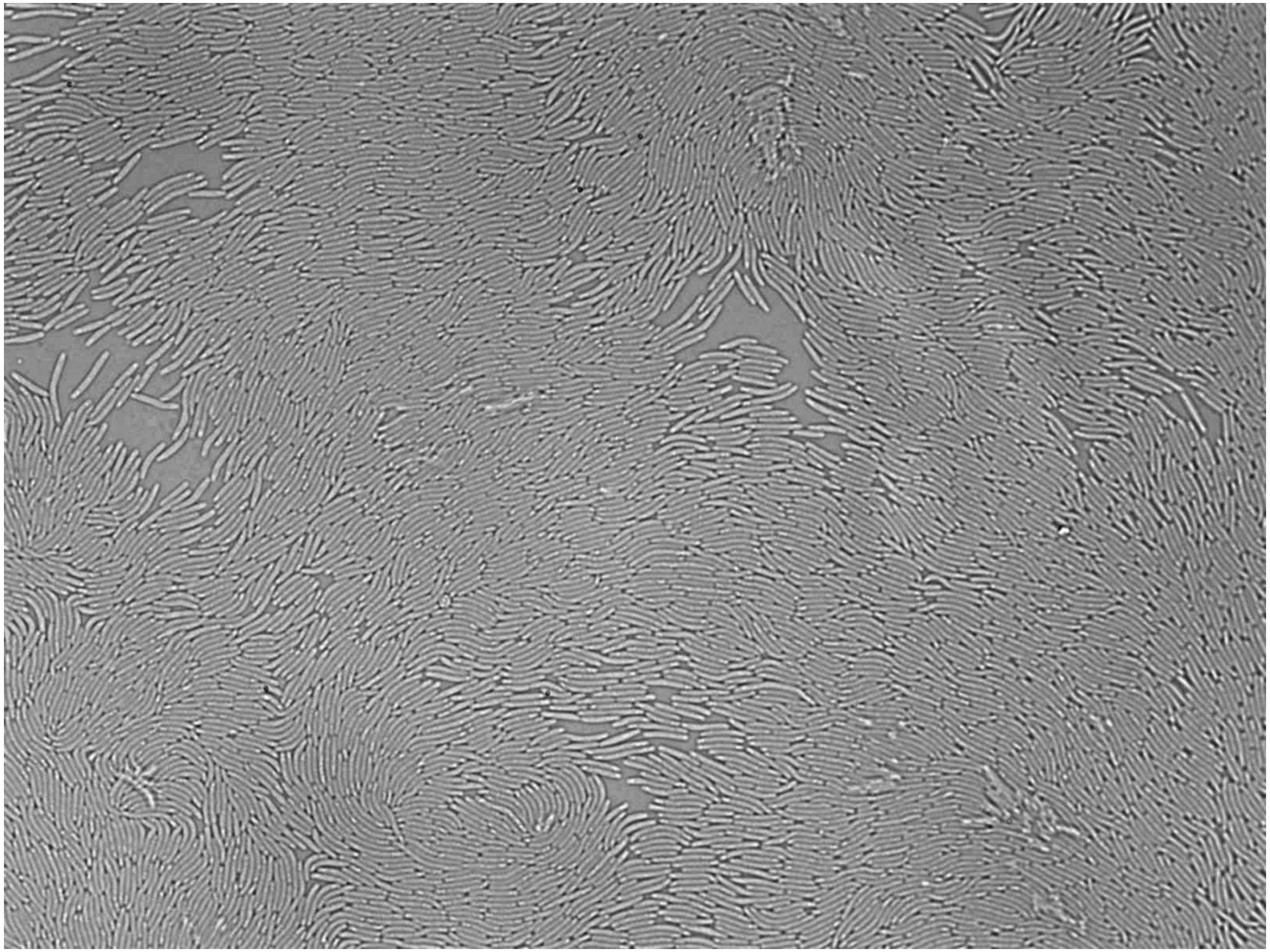
Liquid Crystal Tactoid
Zannoni and coworkers
Soft Matter 2012

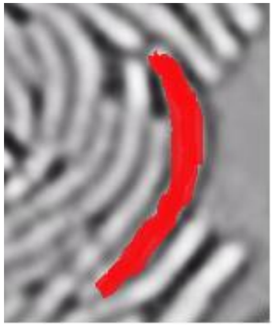


How faceted liquid droplets grow tails
Sloutskin and collaborators
PNAS 2015

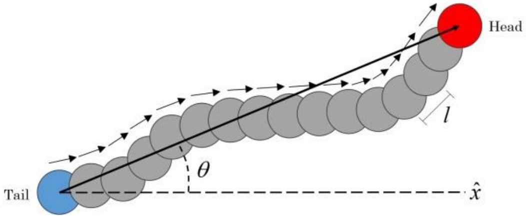
Modeling Flexible Active Nematics

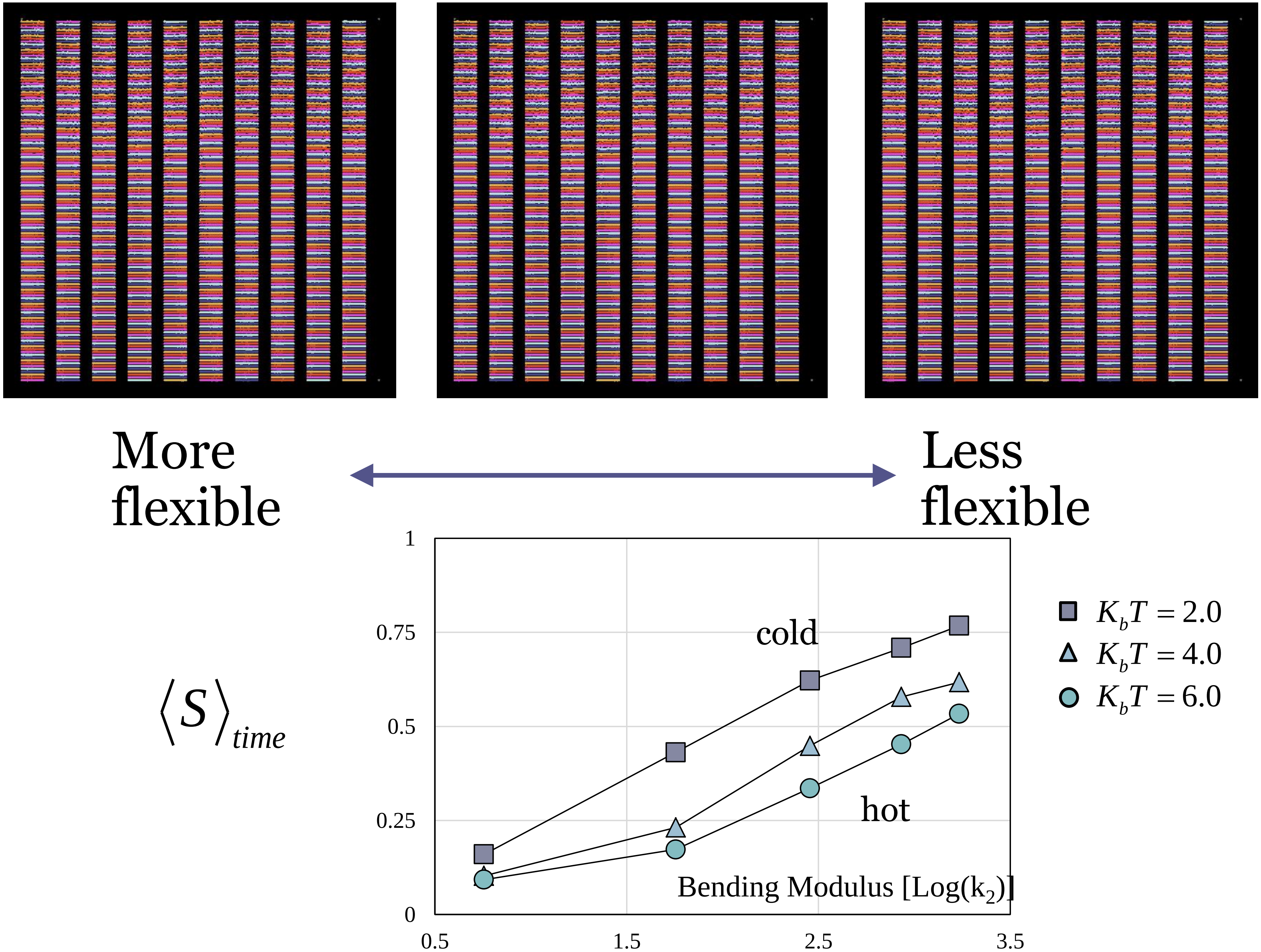
Myxobacteria glide over a surface- Igor Aronson, Argonne Natl Lab

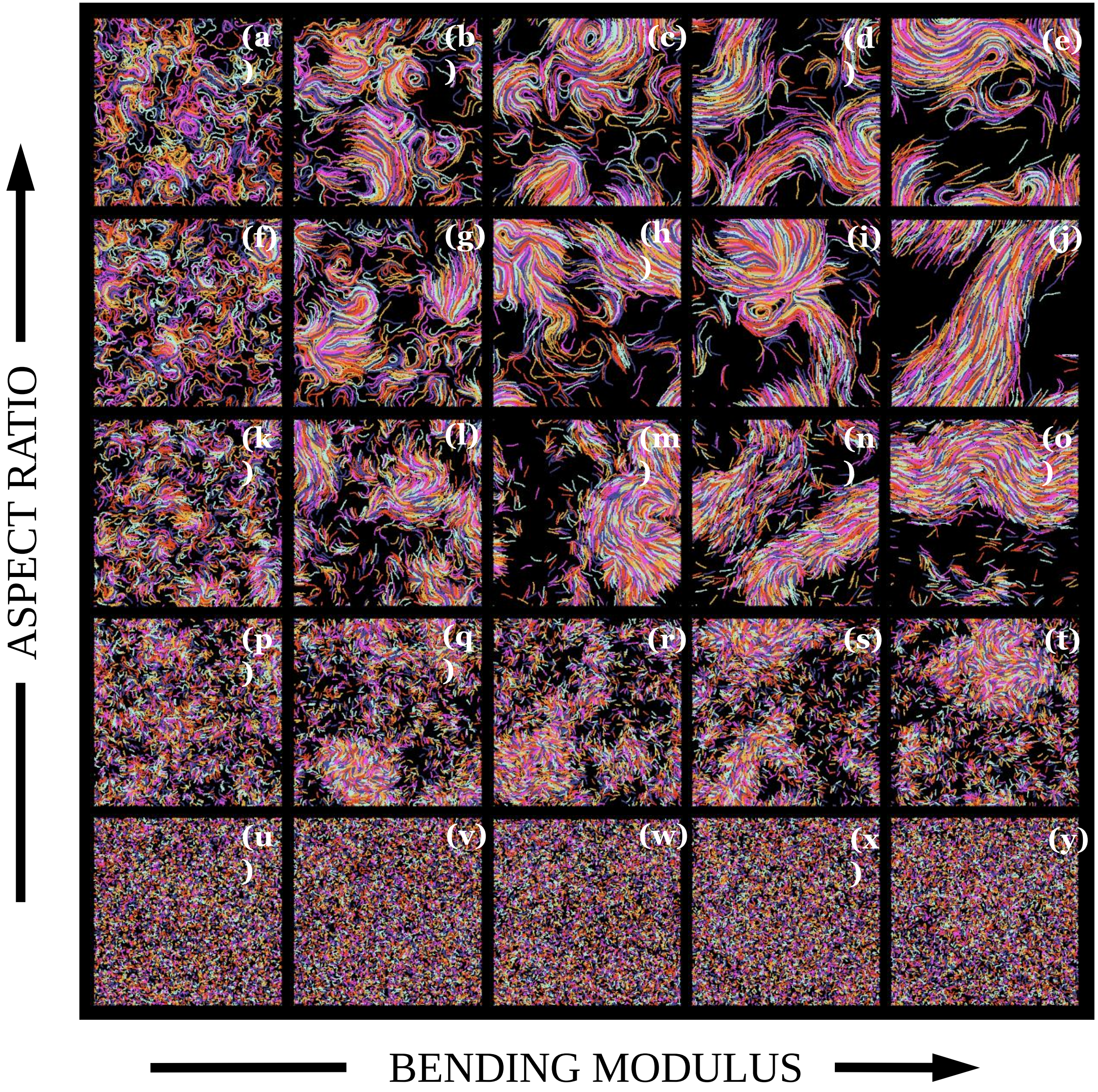




Flexible nematogen

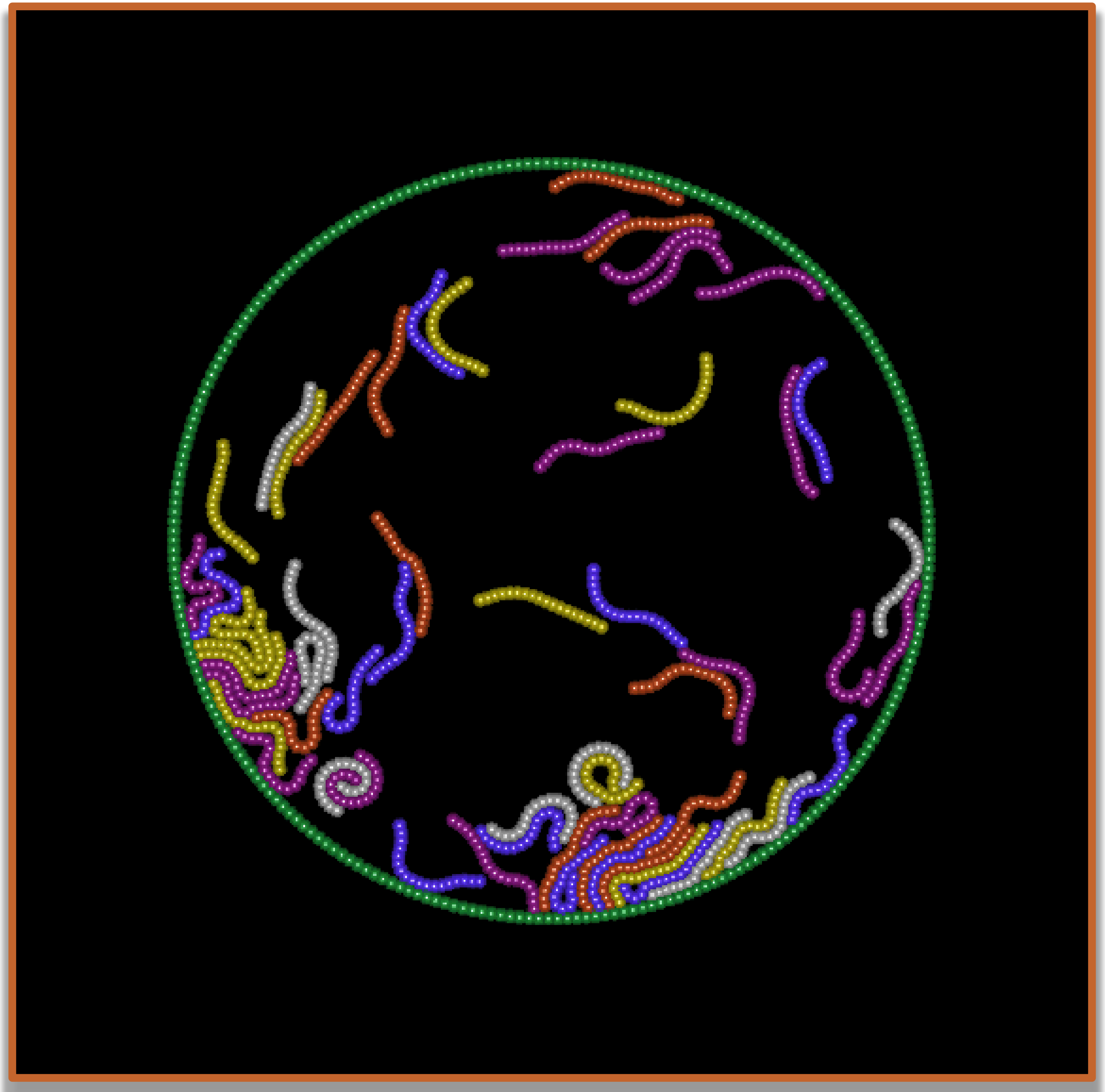


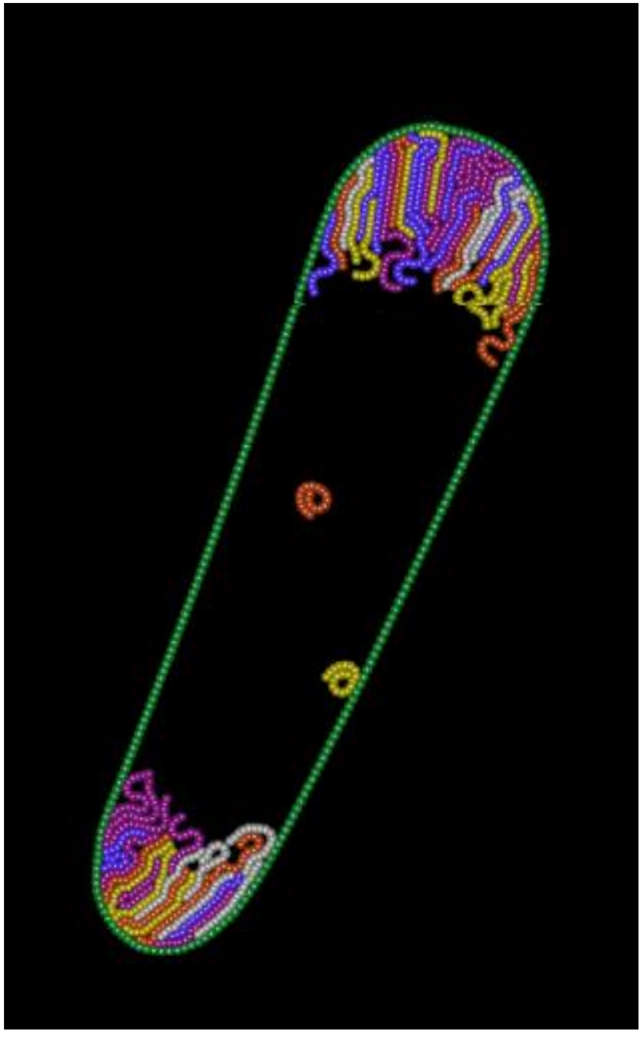

More flexible
Less flexible
$\langle S \rangle_{time}$
1
0.75
0.5
0.25
0
0.5
1.5
2.5
3.5
cold
hot
Bending Modulus [Log(k_2)]
$K_b T = 2.0$
$K_b T = 4.0$
$K_b T = 6.0$


(a)
(b)
(c)
(d)
(e)
(f)
(g)
(h)
(i)
(j)
(k)
(l)
(m)
(n)
(o)
(p)
(q)
(r)
(s)
(t)
(u)
(v)
(w)
(x)
(y)
ASPECT RATIO
BENDING MODULUS

Long "worms," highly flexible → +1 defects

Self propelled particles confined in a flexible container





“Safety pin” structure formed by spontaneous polar segregation

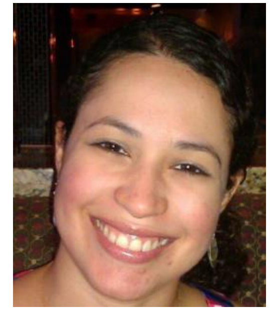
Beating looks like cilia
(though no fluid interactions included!)

Students:

Andrew Konya
(remesh.org)

Mike Varga

Sajedeh Afghah



Vianney Gimenez-Pinto
(Columbia Univ.)

Badel Mbanga
(Univ. of Pittsburgh)

Collaborators:

Jonathan Selinger
Kent State

Linda Hirst
UC Merced

Qi-huo Wei
Kent State

Kenji Urayama
Kyoto

Dick Broer
Eindhoven

Complete list of references: tiny.cc/rselinger2016

Funding: NSF

NSF-DMR 1409658 and 1106014
NSF-CMMI 1436565

Conclusions

Engineering design of complex actuators requires accurate modeling tools

Solved: the "forward problem"
...Determine shape transformation driven by a prescribed director microstructure

Next theoretical challenges:

1st inverse problem: Design a director microstructure that drives target shape transformation

2nd inverse problem: Design surface patterns to blueprint desired 3-d microstructure

Model mechanics and dynamics of light actuation

Goal: programmable materials for actuators, robotics and manufacturing

NSF-DMR 1106014, NSF-DMR 1409658, and NSF CMMI-1436565

References: tiny.cc/selinger2016

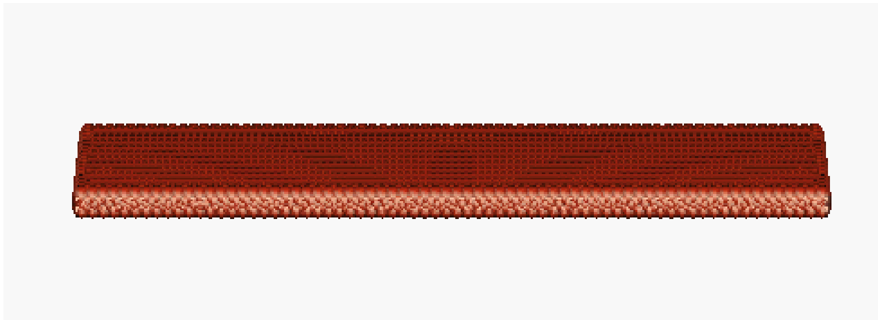
Open invitation to experimenters: we can model your experiment
Open invitation to theorists: we'll teach you our FEM algorithm

Extra slides

Complex Twisted Director: Accordion actuator

FEM - High-*T* range – ΔS=-0.6

Side view



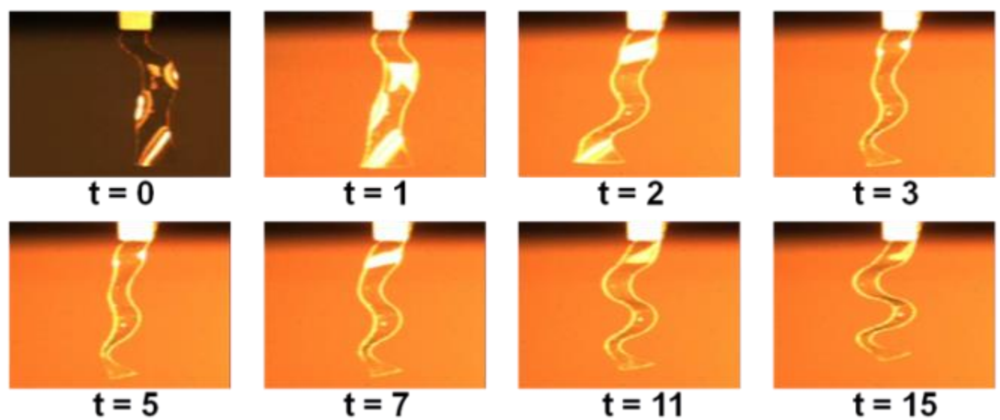
Top view

Oscillating shape with chiral crests and valleys.

Borders form a zigzag due to the chiral bending.

Chirality due to the handedness of director twist.

Experimental Study by De Haan



Aspect ratio: 500-100-10

X-geometry: How Shape depends on θ?

Y. Sawa, et al. Phys. Rev. E 88, 022502 (2013)

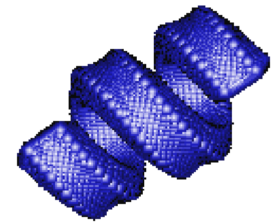
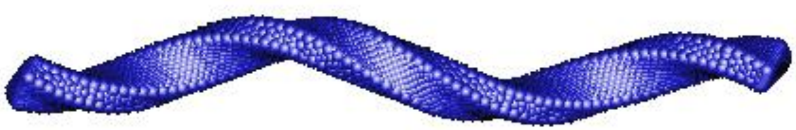
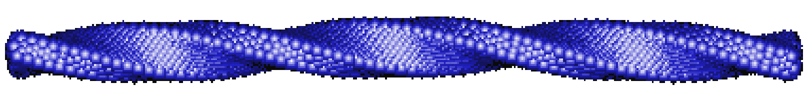
Equilibrium shape of TNE-X with different θ

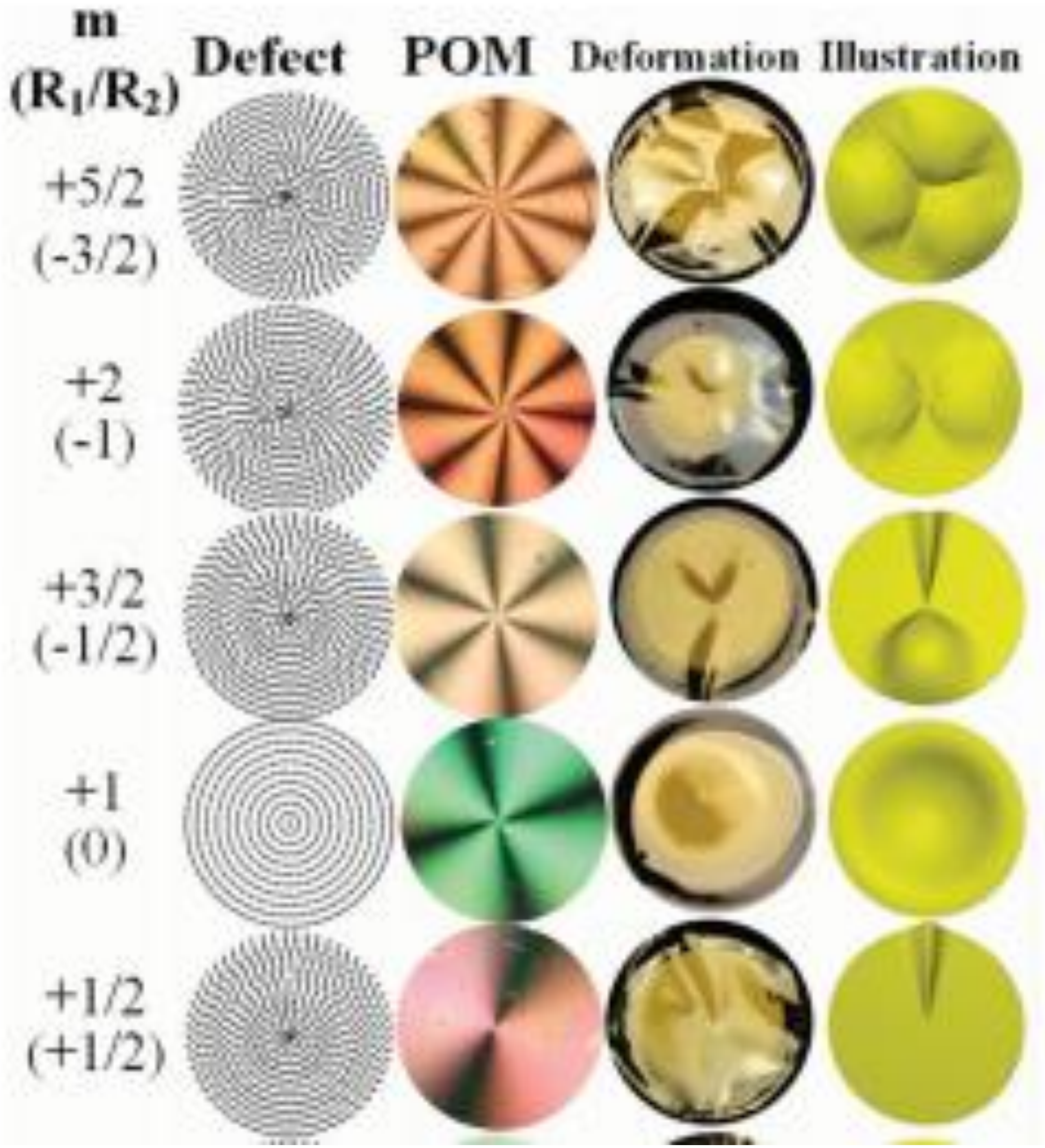
Spiral Ribbon

Intermediate states:

Coexistence of spiral and helicoid twist

Helicoid Ribbon
S-geometry

θ	Equilibrium State T/T_{NI}=1.01
-5°	
-15°	
-25°	
-35°	
-45°	

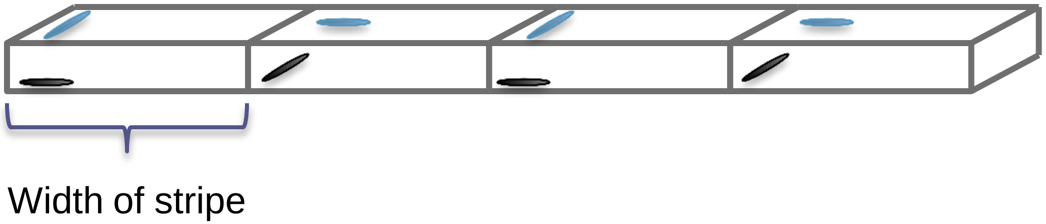


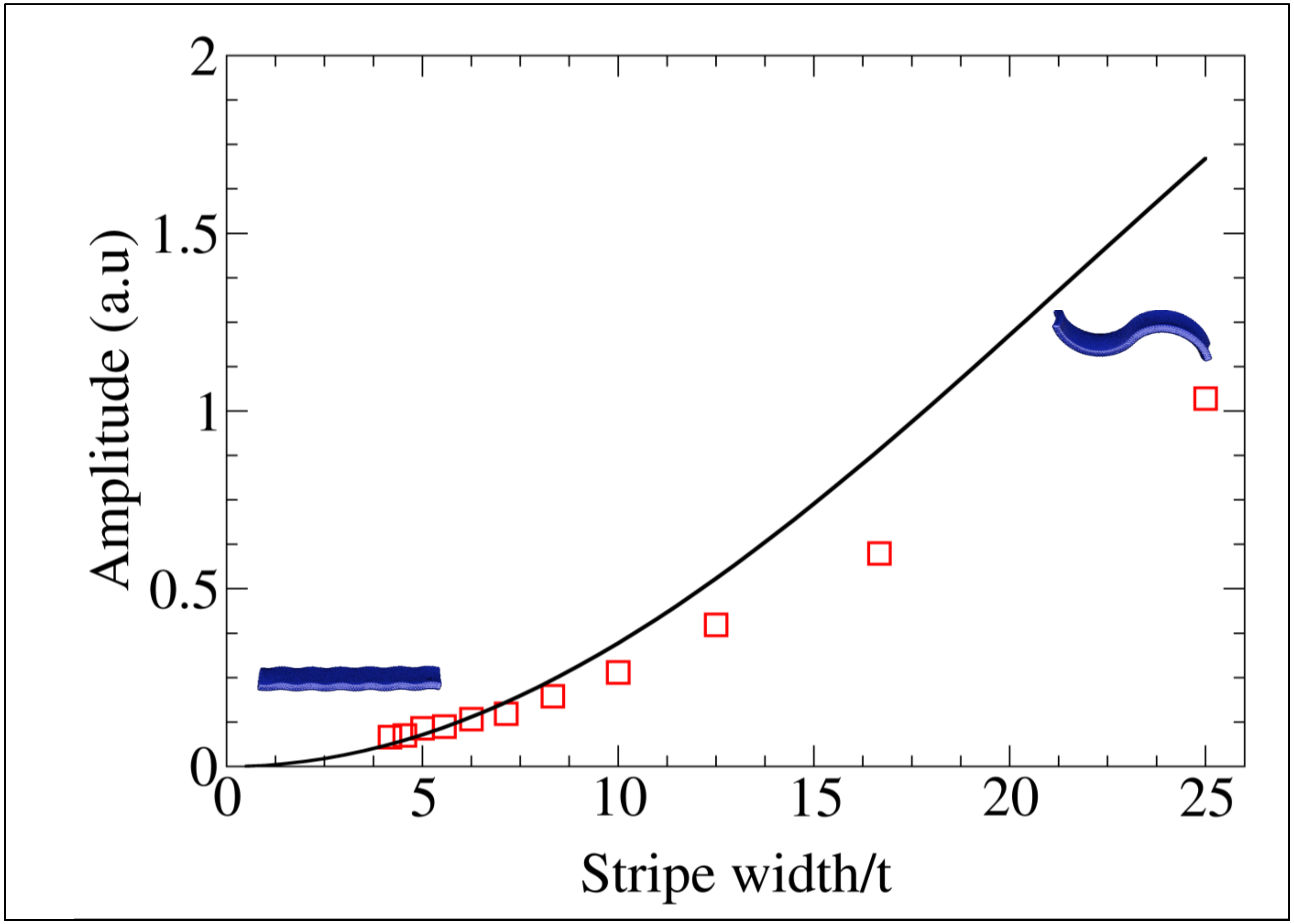
"Topography from Topology" McConney et al

Advanced Materials 2013

Blueprinted glassy nematic films with high order +, - defects

Complex Twisted Director: Accordion actuator





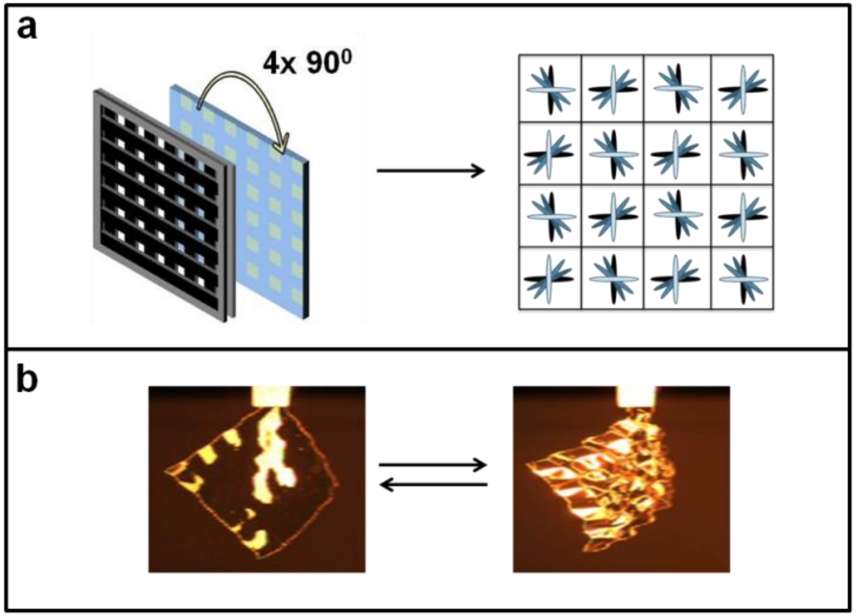
For narrower stripe width:

- Shorter wavelength
- Amplitude is smaller

Aspect ratio: 500-100-10

Checkerboard domains

Collaboration with Eindhoven group

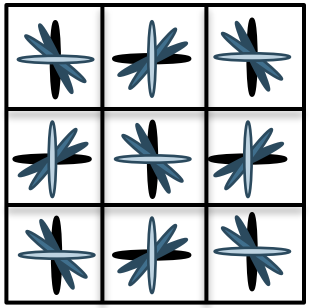


Each square domain bends, upward or downward depending on director twist

Creates "egg-crate" bumps and depressions

LT de Haan, V Gimenez-Pinto, A Konya, TS Nguyen, JMN Verjans, C Sánchez-Somolinos, JV Selinger, RLB Selinger, Dirk Broer, APHJ Schenning
Advanced Functional Materials 2014

FEM simulations



a

b

Aspect ratio
500:150:10

Initial state: nematic director twisted, S-geometry
Gradually drop scalar order parameter to zero
Add dissipation, slightly underdamped ➔
HELICOID