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

Robin Selinger

Kent State will host International Liquid Crystal Conference
ILCC 2016

*** Abstracts due Feb 29 ***
First synthesized by Finkelmann group in 1991

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

Temperature
B. Ratna and J. Naciri
Naval Research Laboratory

Photoexcitation
TJ White et al
AFRL
Actuation mechanisms

Nematic elastomer

Raise Temperature

Isotropic

Nematic+azo dye

Photoexcitation

trans $\rightarrow$ cis

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...

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

Elastic potential energy
(Nonlinear: Green-Lagrange strain)

\[ U_{\text{potential}} \]

Kinetic energy
(lumped mass approximation)
Nodes move via $f = ma$ 

$$\ddot{r}_n = -\frac{\partial U_{pot}}{\partial r_n}$$

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...

\[ \vec{n}^o = \text{blueprinted director} \]

\[ Q_{ij} = \frac{1}{2} \left( 3n_in_j - \delta_{ij} \right) \]

\[ Q_{ij}^0 \rightarrow \text{Describes nematic order at cross-linking defined in each volume element} \]

\[ Q_{ij} = S(T)Q_{ij}^0 \rightarrow S = \text{scalar order parameter, drops on heating} \]

- S=1 perfect nematic order
- S=0 isotropic

Scalar order parameter drops with temperature
\[ H = \sum_{\text{elements } n} \left[ \frac{1}{2} C_{ijkl} \varepsilon_{ij}^n \varepsilon_{kl}^n - \alpha \left( Q_{ij} - Q_{ij}^0 \right) \varepsilon_{ij}^n \right] V_n + \sum_{\text{nodes } p} \left[ \frac{1}{2} m_p v_p^2 \right] \]

- **Elastic potential energy** \( U_{\text{pot}} \)
- **Couples strain and nematic order**
- **Kinetic energy**

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

Changing \( Q_{ij} \) changes the local metric \( \rightarrow \) shape change
Modes and Warner predicted:

\[ T > T_{\text{flat}} \text{ (high } T \text{ range)} \]

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

Sample aspect ratio 50:1
Heat uniformly...
Up-down symmetry $\rightarrow$ metastable state

-4 defect

Heat from one side $\rightarrow$ 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

Nematic director twists 90° from bottom to top

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

<table>
<thead>
<tr>
<th>Aspect ratio</th>
<th>Equilibrium shape</th>
<th>L geometry</th>
<th>S geometry</th>
</tr>
</thead>
<tbody>
<tr>
<td>50-5-1</td>
<td>Helicoid ribbon</td>
<td><img src="image1" alt="L geometry" /></td>
<td><img src="image2" alt="S geometry" /></td>
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<td>50-10-1</td>
<td>Helicoid ribbon</td>
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<td>50-25-1</td>
<td>Spiral ribbon</td>
<td><img src="image9" alt="L geometry" /></td>
<td><img src="image10" alt="S geometry" /></td>
</tr>
</tbody>
</table>

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
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

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

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*

\[ Q_{ij} = q e^{i(kx - wt)} \begin{bmatrix} 1 & 0 & 0 \\ 0 & -0.5 & 0 \\ 0 & 0 & -0.5 \end{bmatrix} \]
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*

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**Burke et al**
*Soft Matter 2015*

**RLBS, A Konya, Al, and JV Selinger**

**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

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

Morphology change
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

$\langle S \rangle_{\text{time}}$

Less flexible

$K_b T = 2.0$
$K_b T = 4.0$
$K_b T = 6.0$

Bending Modulus [Log($k_2$)]
Long “worms,” highly flexible $\rightarrow$ +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

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- 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 – \(\Delta S = -0.6\)

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
Equilibrium shape of TNE-X with different $\theta$

Spiral Ribbon

Intermediate states:
Coexistence of spiral and helicoid twist

Helicoid Ribbon

$S$-geometry

<table>
<thead>
<tr>
<th>$\theta$</th>
<th>Equilibrium State $T/T_N=1.01$</th>
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</thead>
<tbody>
<tr>
<td>$-5^\circ$</td>
<td></td>
</tr>
<tr>
<td>$-15^\circ$</td>
<td></td>
</tr>
<tr>
<td>$-25^\circ$</td>
<td></td>
</tr>
<tr>
<td>$-35^\circ$</td>
<td></td>
</tr>
<tr>
<td>$-45^\circ$</td>
<td></td>
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“Topography from Topology”
McConneyey 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
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
Initial state: nematic director twisted, S-geometry
Gradually drop scalar order parameter to zero
Add dissipation, slightly underdamped $\rightarrow$ HELICOID

Aspect ratio
500:150:10