Bending the Rules

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Layered Systems
Cubic Phases
Curvature & Topology
New Focal “Conics”

RDK and T. Lubensky, *PRL* **82** (1999) 2892

[Website Link] www.physics.upenn.edu/~kamien/
Smectic-A Liquid Crystals and Lamellae

Smectic  Two-dimensional fluid / One-dimensional crystal
  A  Molecules normal to layers
  C  Molecules tilt with respect to layer normal

http://www2.sfu.ca/chemistry/faculty/Williams/phasetypes.html
http://www.ch.ic.ac.uk/liquid_crystal/lamellar%20phases.htm
B4 Liquid Crystalline Phase: Bent Layers

Data Courtesy of Noel Clark

bent core or banana molecules
Noel Clark’s Suggestion (and pictures)

“molecules favor negative Gaussian curvature”


oily tails turn to pack
Two Kinds of Curvature

Gaussian or Intrinsic Curvature
\[ K = \kappa_1 \kappa_2 \]

Mean or Extrinsic Curvature
\[ H = \frac{1}{2} (\kappa_1 + \kappa_2) \]

\[ H > 0 \]
\[ K > 0 \]

\[ H = 0 \]
\[ K = 0 \]

\[ H < 0 \]
\[ K < 0 \]
Free Energy and Rotational Invariance

\[ \Phi = 2a \]

\[ \Phi = a \]

\[ \Phi = 0 \]

\[ \rho \propto \cos \left( \frac{2\pi \Phi(r)}{a} \right) \]

\[ \mathbf{n} = \frac{\nabla \Phi}{|\nabla \Phi|} \]

Phase: \[ \Phi = z - u(r) \]

\[ F = \frac{1}{2} \int d^3x \left\{ \left[ \partial_z u - \frac{1}{2} (\nabla u)^2 \right]^2 + K_1 (\nabla \cdot \mathbf{n})^2 \right\} \]

\[ \propto (\nabla \Phi)^2 - 1 \]

Corrections ensure rotational invariance
Nematic Liquid Crystals: Frank Free Energy

\[
F = \frac{1}{2} \int d^3x \left\{ K_1 (\nabla \cdot \mathbf{n})^2 + K_2 [\mathbf{n} \cdot (\nabla \times \mathbf{n}) + q_0]^2 + K_2 [\mathbf{n} \times (\nabla \times \mathbf{n})]^2 \right\}
\]

spontaneous twist

\[
\begin{align*}
\text{Splay} & : \nabla \cdot \mathbf{n} \\
\text{Twist} & : \mathbf{n} \cdot (\nabla \times \mathbf{n}) \\
\text{Bend} & : \mathbf{n} \times (\nabla \times \mathbf{n})
\end{align*}
\]
Saddle Splay

\[ F_{SS} = K_{24} \int d^3x \nabla \cdot [(n \cdot \nabla) n - n (\nabla \cdot n)] \]

\[ F_{SS} = -2K_{24} \int a_n dn \int \sqrt{g_n} d^2\sigma K_n \]
Half the Way with Gauss-Bonnet

\[ \int KdS = 4\pi (1 - g) \]

Handles produce positive saddle-splay

see, for instance, RDK, Rev. Mod. Phys. 74 (2002) 953
Gaussian Curvature Leads to Mean Curvature

\[ R' = R + a \]
\[ \kappa'_i = \frac{\kappa_i}{1 + a\kappa_i} \]

\[ H' = \frac{H + aK}{1 + 2aH + a^2K} \]
\[ K' = \frac{K}{1 + 2aH + a^2K} \]

Differential Form

\[ \mathbf{n} \cdot \nabla H = K - 2H^2 - \frac{1}{2} R_{nn} \]
\[ \mathbf{n} \cdot \nabla K = -2KH \]
Smectics with Cubic Symmetry

Chiral series FH/FH/HH-nBTMHC

Data From Oriented Samples

- Symmetry
  - \( BP_{Sm(A)} \): Cubic
  - \( BP_{Sm(C)} \): Hexatic
  - \( BP_{Sm} 2 \): Orthorhombic
  - \( BP_{Sm} 3 \): Amorphous

- Length scales
  - Layering: \( 4nm \)
  - Persistence: \( 50nm \)
  - Unit Cell: \( 200nm \)

Minimal Surfaces

Schwartz P  Diamond

Neovius  Gyroid

© 1998, James T. Hoffman and MSRI
Aside: Blue Phases


double twist tubes

into lattices

with defects

assemble

*from Liquid Crystals: Nature's Delicate Phase of Matter by Peter J. Collings, Princeton University Press, 1990*
Aside: Blue Phases with Splay Instead of Twist

Grelet, Pansu, Li, and Nguyen, *PRE* 65 (2002) 050701

Our Construction

- Start with P-surface
- Layer inside with dilated unit cells
- Fill with cylinders
- Outside = inside

Stability of P-Phase Relative to Flat Phase

Stability Diagram for 50 layer cell

\[ \lambda \sqrt{2/a} \]

\[ \lambda = \sqrt{\frac{K_1}{B}} \]

\[ |K_{24}|/K_1 \]

layer spacing = a

DiDonna and RDK, PRL 89 (2002) 215504
Structure Function: Model vs. Experiment

- P surface
- x-ray peaks
- Grelet and Pansu

peaks are along the umbilics (flat spots)

DiDonna and RDK, *PRE* 68 (2003) 041703
Many, Many Surfaces to Choose From

- Schoen’s Batwing
- Schoen’s I-WP Surface
- Schoen’s C27(P) Surface
- Schoen’s unnamed Surface 14
- Neovius Surface

Images from Ken Brakke’s Surface Evolver webpage:
http://www.susqu.edu/facstaff/b/brakke/evolver/evolver.html
I-Wp surface

x-ray peaks

Grelet and Pansu

peaks are along the umbilics (flat spots)
I-Wp Construction Very Complicated

I-Wp Construction Very Complicated

- best guess from translating walls normal to themselves.
- prefers 1/2 defect lines
- planes, cylinders and minimal surfaces
- genus = 7, more than twice P surface

DiDonna and RDK, PRE 68 (2003) 041703
Hopeless!

Data Courtesy of Noel Clark

bent core or banana molecules
More General Approaches

Topological Defects
- nonlinear elasticity
- solitons and linear superposition
- evolution by advection

Even Spacing (Foliation)
- focal conic domains
- curved backgrounds
Topology and Nonlinear Elasticity

\[ F = \frac{B}{2} \int d^3x \left\{ \left[ \partial_z u - \frac{1}{2} (\nabla u)^2 \right]^2 + \lambda^2 (\nabla \cdot n)^2 \right\} \]

Long wavelength bends & small compression strain:

Harmonic: \[ F = \frac{B}{2} \int d^3x \left[ (\partial_z u)^2 + \lambda^2 (\nabla^2_u)^2 \right] \]

Nonlinear enough (i.e. shows anomalous elasticity\(^\dagger\)): \[ F = \frac{B}{2} \int d^3x \left\{ \left[ \partial_z u - \frac{1}{2} (\nabla^2_u)^2 \right]^2 + \lambda^2 (\nabla^2_u)^2 \right\} \]

\(^\dagger\) à la Grinstein and Pelcovits, PRL 47 (1981) 856
Edge Dislocations

\[ \partial_z u - \frac{1}{2} (\nabla \perp u)^2 = \lambda \nabla^2_{\perp} u \]

\( b \ll \lambda \)  

Harmonic Theory

Ishikawa and Lavrentovich, *PRE* 60 (1999) R5037


compression = bending

fits all the layers
Why does this work?

\[ F = \frac{B}{2} \int d^3x \left\{ \left[ \partial_z u - \frac{1}{2} (\nabla \nabla u)^2 - \lambda \nabla^2 u \right]^2 + \frac{4\lambda}{3} K u + \lambda \nabla \cdot A \right\} \]

\[ \bar{K} = \frac{1}{2} \nabla \cdot [\nabla \nabla u - (\nabla u \cdot \nabla) \nabla u] \]

\[ A = - (\nabla u)^2 \hat{z} + 2 \partial_z u \nabla u - \frac{1}{3} (\nabla u)^2 \nabla u + \frac{2}{3} u (\nabla \psi + \hat{z} \times \nabla \phi) \]

BPS Solutions

Hopf-Cole

\[ u = 2\lambda \ln S \]

\[ \partial_z S = \lambda \nabla^2 S \]

superposition principle!

Prasad and Sommerfield, PRL 35 (1975) 760

Santangelo and RDK, PRL 91 (2003) 045506
Interaction Energy of Dislocations: Edge versus Screw

tilt grain boundary

\[ F = \frac{B\lambda}{2} \int A \cdot dS \]
\[ \hat{z} \cdot A = - (\nabla_\perp u)^2 = \hat{z} \cdot A_{\text{linear}} \]

exponential interactions

Santangelo and RDK, *PRL* 91 (2003) 045506

twist grain boundary

a.k.a. Scherk’s first surface

superposition principle!


power-law interactions

RDK and T. Lubensky, *PRL* 82 (1999) 2892
Evolution of the Skeletal Graph

\[
\Gamma \equiv \partial_z u - \frac{1}{2} (\nabla_\perp u)^2 - \lambda \nabla_\perp^2 u = 0
\]

Burgers Equation

\[
v = -\nabla_\perp u \quad \quad \partial_z v + (v \cdot \nabla_\perp) v = \lambda \nabla_\perp^2 v \quad \nabla_\perp \times v = 0
\]

Euler-Lagrange Equation

\[
-\partial_z \Gamma + \nabla_\perp \cdot [(\nabla_\perp u) \Gamma] - \lambda \nabla_\perp^2 \Gamma = -\frac{2}{3} \lambda \bar{K}
\]

\[
\partial_z \Gamma + \nabla_\perp \cdot [v \Gamma] = \lambda \nabla_\perp^2 \Gamma - \frac{2}{3} \lambda \bar{K}
\]

advection with Gaussian Curvature as source

Focal Conic Domains

Dupin cyclides (generalized tori)

equally spaced layers degenerate into ellipses

C. Williams, in De Gennes and Prost, *Liquid Crystals*
Equal Spacing: Higher Genus Focal “Conics”

layered surfaces (generalized polyhedra)

energetically stable

*higher genus means more saddle-splay*

Data Courtesy of Noel Clark

DiDonna and RDK, PRE 68 (2003) 041703
Equal Spacing: Higher Genus Focal “Conics”

hyperbolic octahedra tessellate the hyperbolic plane

Recall
\[ \mathbf{n} \cdot \nabla H = K - 2H^2 - \frac{1}{2} R_{nn} \]
\[ \mathbf{n} \cdot \nabla K = -2KH \]

Einstein manifolds
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