

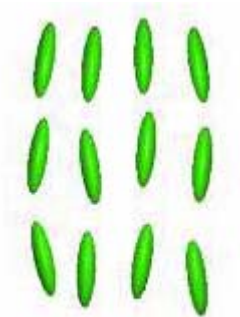
Order Parameters and Defects in Liquid Crystals

Ferroelectric phenomena in liquid crystals

June, 2007

Liquid Crystal-substance with a degree of crystalline order that remains in a liquid state

- Simple picture- long thin molecules



Liquid Crystal

Energy to describe static stable configurations

Made up of competing energies

- Molecular packing (molecular alignment)
- Thermal effects (randomize alignment)
- External stresses (mechanical, electrical..)

Temperature dependent-different terms become dominant at different temperatures

↑
Isotropic

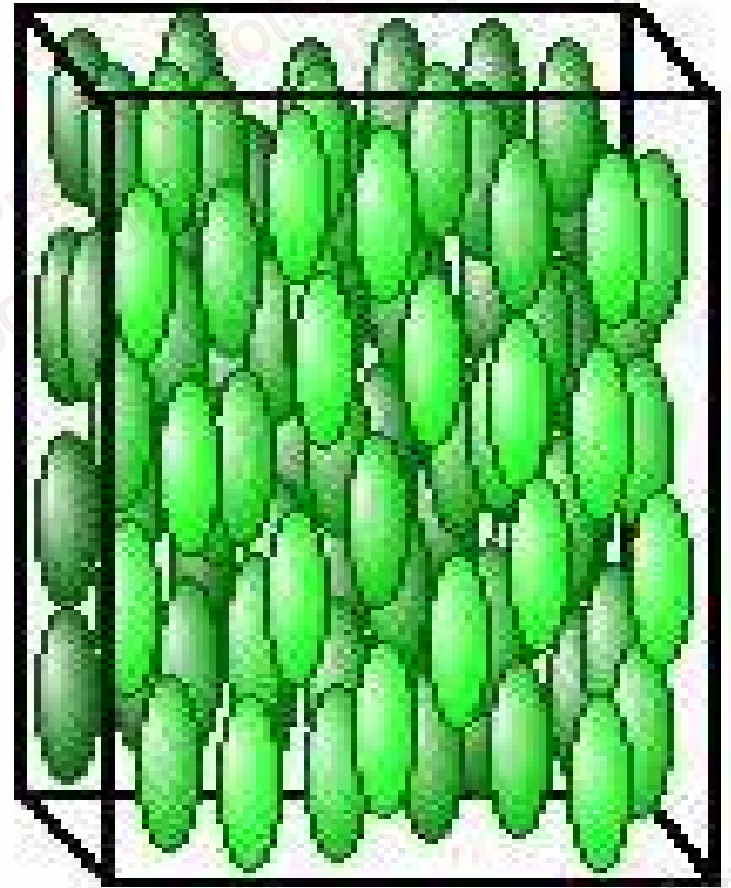
Nematic

Smectic

T

- Nematic phase-energy seeks local alignment of long axes.
- $\mathbf{n}(\mathbf{x})$ is the “local average” of long axes.
- $|\mathbf{n}(\mathbf{x})| = 1$

↑
 $\mathbf{n}(\mathbf{x})$



$\mathbf{n}(\mathbf{x})$ is a unit vector field

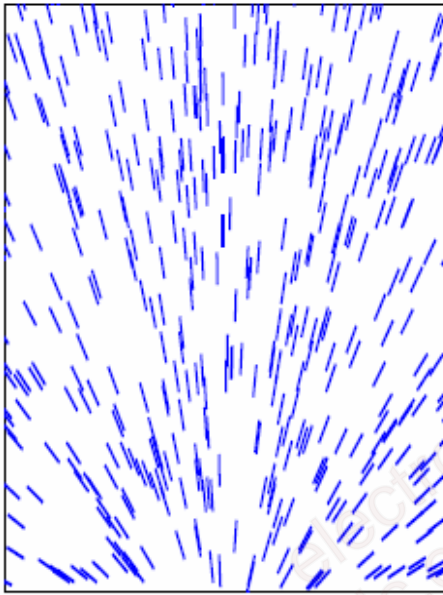
- Molecules do not have a head and tail as $\mathbf{n}(\mathbf{x})$ does.
- In problems where this does not lead to inconsistencies $\mathbf{n}(\mathbf{x})$ is the simplest way to describe a nematic liquid crystal.
- $\mathbf{n}(\mathbf{x})$ -director field

Oseen Frank Energy

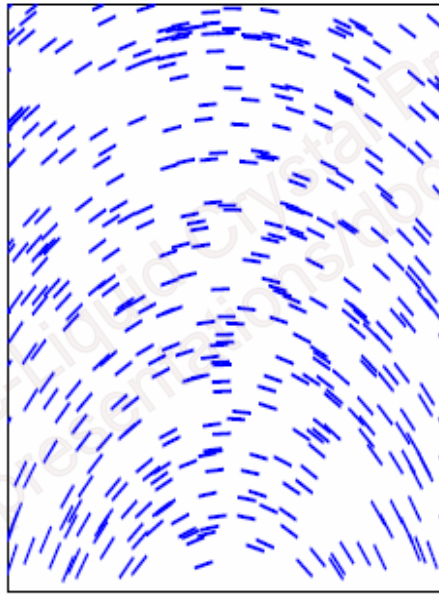
- Energy records the cost of distortions away from $\mathbf{n}(\mathbf{x}) = \text{const.}$
- Written in terms of pure splay, twist, and bend. These have K_1, K_2, K_3 as coefficients respectively

$$F_F(\mathbf{n}) = \int_{\Omega} [K_1(\nabla \cdot \mathbf{n})^2 + K_2(\mathbf{n} \cdot \nabla \times \mathbf{n})^2 + K_3|\mathbf{n} \times \nabla \times \mathbf{n}|^2 + (K_2 + K_4)[\text{tr}(\nabla \mathbf{n})^2 - (\nabla \cdot \mathbf{n})^2]] dx,$$

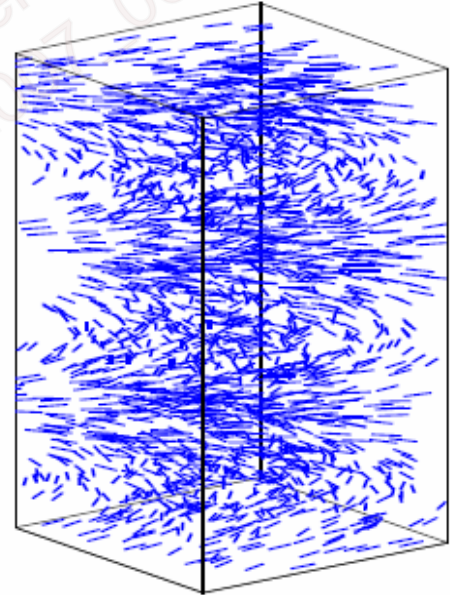
Pure Distortions



Splay



Bend



Twist

Special case, $K_1 = K_2 = K_3 = K$, $K_4 = 0$, one constant approximation

vector identity

$$\text{tr}(\nabla \mathbf{n})^2 - (\nabla \cdot \mathbf{n})^2 = |\nabla \mathbf{n}|^2 - |\nabla \times \mathbf{n}|^2 - (\nabla \cdot \mathbf{n})^2,$$

$$\Rightarrow F_F(n) = \int_{\Omega} K |\nabla \mathbf{n}|^2 d\mathbf{x},$$

Boundary Conditions

1) $n = n_0$ on $\partial\Omega$, $|n_0| = 1$

2) $F_b = c \int_{\partial\Omega} (n \cdot e(x))^2$

1) Strong anchoring problem

2) $F = F_F + F_b$ weak

anchoring

If $c < 0$ then $n(x)$ tends to be parallel to $e(x)$. $e(x)$ is the easy axis.

If $n(x)$ or $e(x)$ are parallel to the boundary normal

we are promoting “homeotropic” boundary values.

If $c > 0$ then $n(x)$ tends to be \perp $e(x)$ on the boundary. If $e(x)$ is parallel to the boundary normal then $n(x)$ tends towards tangential boundary values.

$$F_F(n) = \int_{\Omega} [K_1(\nabla \cdot n)^2 + K_2(n \cdot \nabla \times n)^2 + K_3|n \times \nabla \times n|^2 + (K_2 + K_4)[\text{tr}(\nabla n)^2 - (\nabla \cdot n)^2] dx,$$

Thm

Assume $\partial\Omega$ is a smooth surface, n_0 is smooth, $K_1, K_2, K_3 > 0$.

Then there is a minimizer for $F(n)$ in the class

$$A = \{u \mid u : \Omega \rightarrow S^2, u = n_0 \mid_{\partial\Omega}, \int_{\Omega} |\nabla u|^2 < \infty\}$$

provided A is nonempty.

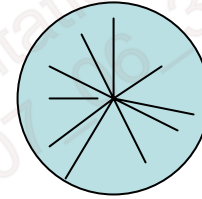
$n(x)$ may have singularities, “defects”

- ex . $n(x) = x/|x|$

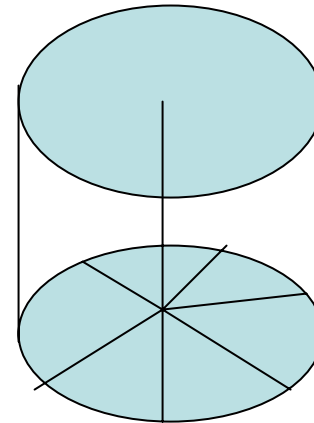
“Hedgehog”. $n(x)$ has homeotropic b.v. and a defect at one point. Minimizers from the theorem can not be singular on a curve. Line singularities in liquid crystals do exist, “disclination lines”.

Try $n(r, \theta, z) = e_r$ and get

$$\int |\nabla n|^2 = \infty$$

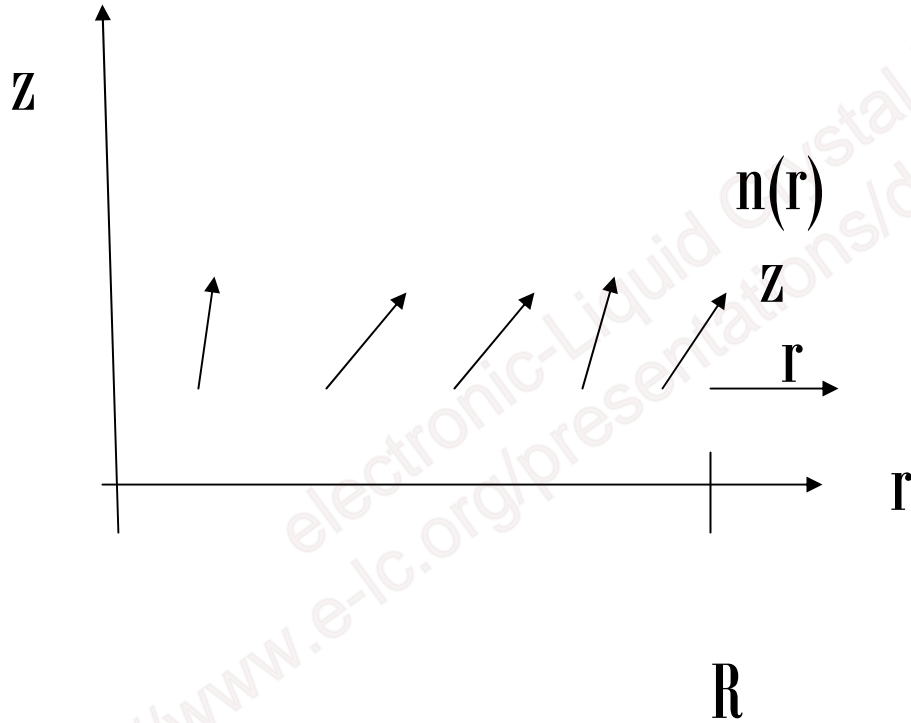


$$\Omega = B_R$$



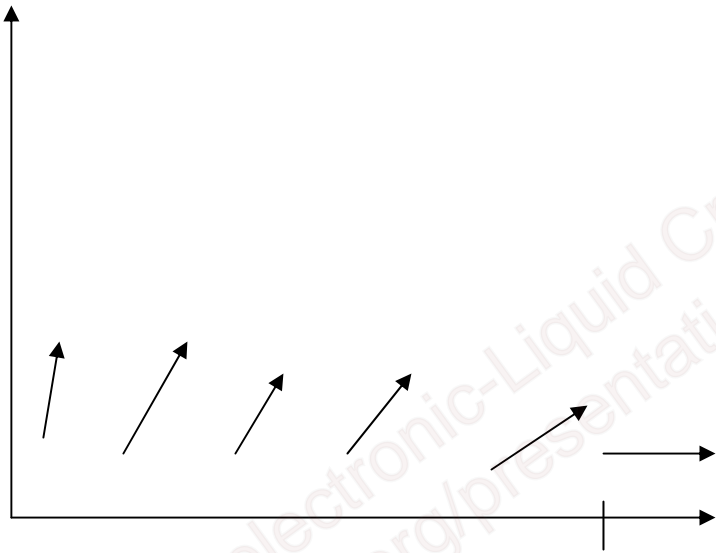
Cladis and Kleman consider :

$$n(r) = \cos \varphi(r) e_r + \sin \varphi(r) e_z \quad \text{with} \quad \varphi(R) = 0$$



$$F = \int_{B_R} |\nabla n|^2 dx dy = 2\pi \int_0^R \left((\varphi')^2 + \frac{\cos^2 \varphi}{r^2} \right) r dr$$

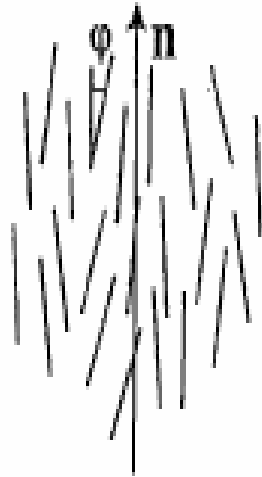
They prove the minimizer is $\varphi(r) = \frac{\pi}{2} - 2 \tan^{-1}\left(\frac{r}{R}\right)$



R

Solution is not singular. It escapes to the third dimension.

Introduce an order parameter that allows n to “melt” near $r=0$



$f(\varphi)$ probability density that the director of molecules near x are within an angle φ of $n(x)$.

$$f_0(\varphi) = \frac{1}{4\pi}$$

$s(x)$ is the isotropic order parameter .

Measures how concentrated f is near $\varphi = 0$.

$$s(x) = \frac{3}{2} \int_{S^2} \cos^2(\varphi) (f - f_0)$$

$s=1$ strongly nematic, $s=0$ isotropic

Ericksen considers a nematic described by the pair (s,n)

$$\int (k |\nabla s|^2 + s^2 |\nabla n|^2) dx$$

http://www.e-lc.org/presentations/docs/2007_06_30_14_00_13

If $k \leq 1$

Mizel, Rocco, and Virga prove that this has a minimizer

(\tilde{s}, \tilde{n}) in the family

$$\{s(r), \cos \varphi(r)e_r + \sin \varphi(r)e_z, \varphi(R) = 0, s(R) = s_0 > 0\}$$

of the form $\tilde{\varphi} \equiv 0, \tilde{s}(r) > 0$ for $r > 0, \tilde{s}(0) = 0$

The solution is allowed to melt into the isotropic phase at $r=0$,

has finite energy, and has a disclination line along the z axis.

If $k > 1$ then the solution has $\tilde{s}(0) > 0$ and $\tilde{\varphi}(0) = \frac{\pi}{2}$.

Defect Core Structure in Nematic Liquid Crystals

N. Schopohl and T. J. Sluckin^(a)

$$F_{\text{bulk}} = A \text{tr} \mathbf{Q}^2 + \frac{2}{3} B \text{Tr} \mathbf{Q}^3 + \frac{1}{2} C \text{Tr} \mathbf{Q}^4,$$

$$F_{\text{kin}} = L_1 \frac{\partial Q_{ij}}{\partial x_k} \frac{\partial Q_{ij}}{\partial x_k} + L_2 \frac{\partial Q_{ij}}{\partial x_j} \frac{\partial Q_{ik}}{\partial x_k} + L_3 \frac{\partial Q_{ij}}{\partial x_k} \frac{\partial Q_{ik}}{\partial x_j},$$

$$Q_{ij} = Q_{ji} \text{ and } \text{tr} \mathbf{Q} = 0$$

The full free-energy functional

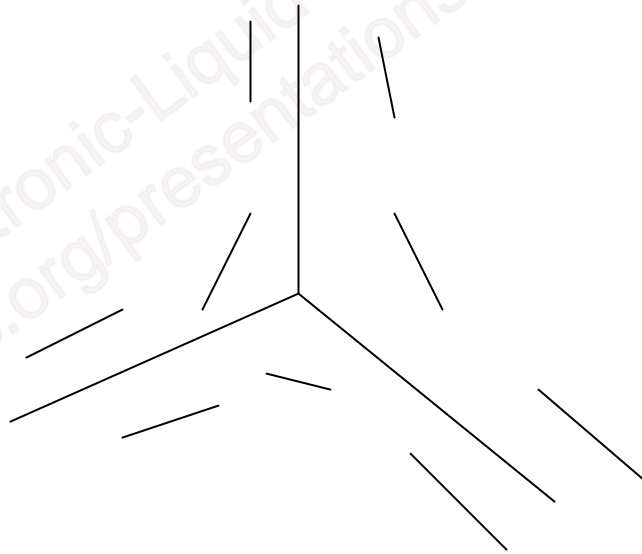
$$F(\mathbf{Q}, \mathbf{\Lambda}) = F_{\text{bulk}} + 2 \text{tr}(\mathbf{\Lambda} \mathbf{Q}) + F_{\text{kin}}$$

uniaxial

$$\mathbf{Q} = s(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3}\mathbf{I})$$

biaxial

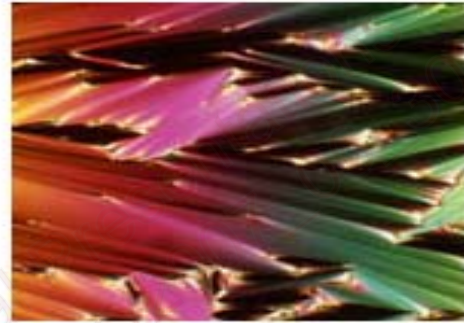
$$\mathbf{Q} = -(s_1\mathbf{n} \otimes \mathbf{n} + s_2\mathbf{m} \otimes \mathbf{m}) + \frac{1}{3}(s_1 + s_2)\mathbf{I},$$



Smectics



Picture of the smectic A phase



*Photo courtesy of
Dr. Mary Neubert LCI-KSU*

Photo of the smectic A phase
(using polarizing microscope)



Picture of the smectic C phase

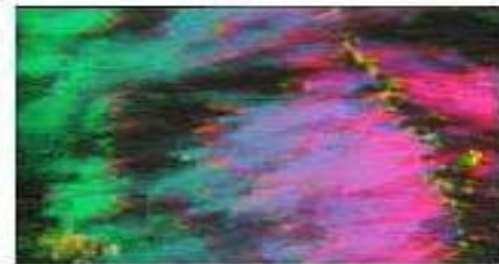


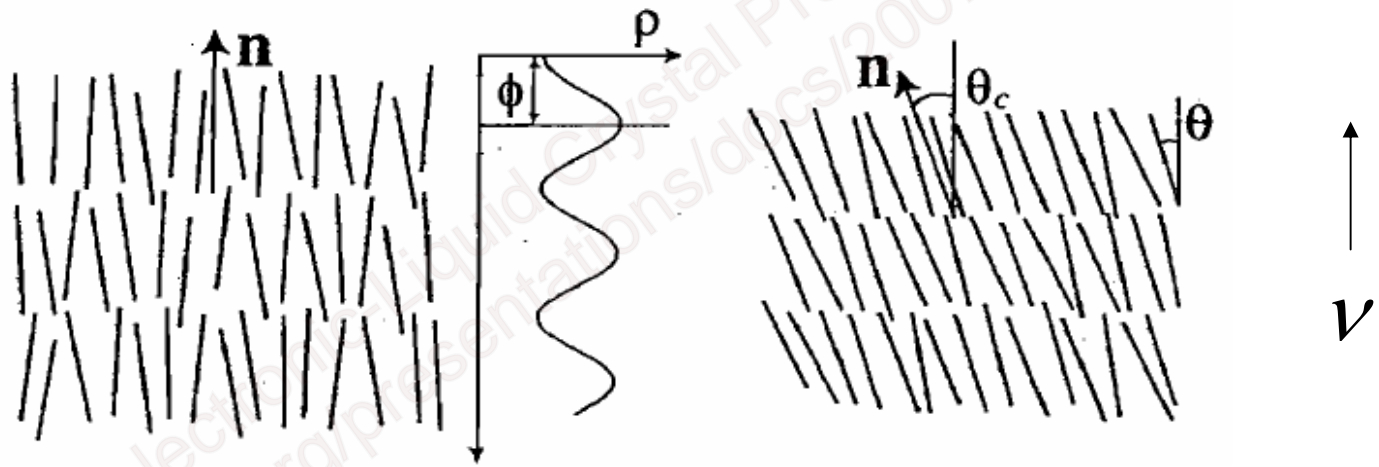
Photo courtesy Dr. Mary Neubert LCI-KSU

Photo of the smectic C phase
(using polarizing microscope)

<http://www.electrofluids.com/Liquid-Crystals/Smectic-Phases>

14_00_13

Molecules locally align and in addition form layers



- Layer normal \mathbf{V}

- Density modulation

$$\rho(x) = \rho_0 + \rho_1 \cos\left(\frac{2\pi}{d} \mathbf{V} \cdot \mathbf{x}\right)$$

- $q = \frac{2\pi}{d}$, d = layer thickness
- If $\rho_1 > 0$ then layers exist - smectic phase
- If $\rho_1 = 0$ then no layers - nematic phase

- If $v \parallel n$ - smectic A
- If not - smectic C
- Complex order parameter

$$\psi = \rho(x)e^{i\varphi(x)}$$

$$2\rho_1 \cos \varphi = \psi + \psi^*$$

- $\psi = 0$ nematic, $\psi \neq 0$ smectic

Energy

$$F_A = |(i\nabla + q\mathbf{n})\Psi|^2 + A(1 - |\psi|^2)^2$$
$$|\nabla\rho_1|^2 + \rho_1^2 |\nabla\varphi - qn|^2 + A(1 - \rho_1^2)^2$$

III

II

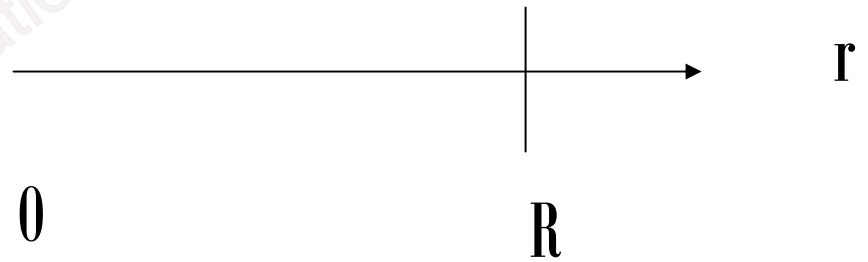
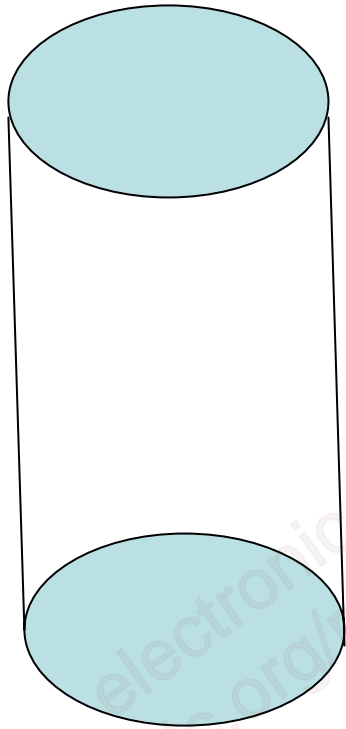
I

$$A > 0$$

- I $\rho_1 = 1$ prefers smectic phase
- II locally the level sets of φ are the layers, $\nabla\varphi \parallel n$, $|\nabla\varphi| \approx q$
- III penalizes phase transitions

Smectic-*A* structures in submicrometer cylindrical cavities

S. Kralj^{1,2} and S. Žumer²



http://www.e-ic.org/electronic-Liquid-Crystal-Presentations/docs/2007_06_30_14_00_13

$$f = f_n^{\text{loc}} + f_n^{\text{non}} + f_s^{\text{loc}} + f_s^{\text{non}}$$

$$f_n^{\text{loc}} = A(T - T^*)S^2 - BS^3 + CS^4,$$

$$f_n^{\text{non}} = \frac{K_{11}(\text{div}\vec{n})^2}{2} + \frac{K_{22}(\vec{n} \cdot \text{curl}\vec{n})^2}{2} + \frac{K_{33}(\vec{n} \times \text{curl}\vec{n})^2}{2} \\ + L(\text{grad}S)^2,$$

$$f_s^{\text{loc}} = a(T - T_{NA})|\tilde{\psi}|^2 + \frac{b|\tilde{\psi}|^4}{2},$$

$$f_s^{\text{non}} = C_{\parallel}|(\vec{n} \cdot \text{grad} - iq_0)\tilde{\psi}|^2 + C_{\perp}|(\vec{n} \times \text{grad})\tilde{\psi}|^2,$$

$$f_{\text{surf}} = -\frac{S}{2}(\vec{n} \cdot \vec{e}_{\text{easy}})^2$$

$$\int_0^R f r dr + f_{\text{surf}} R$$

$$K_{ii} = S^2 k_{ii},$$

$$e_{easy} = e_r$$

IV. STRUCTURES—Sm-*A* PHASE

Based on the “nematic” history we propose five qualitatively different smectic structures which are allowed from the topological point of view. According to their appearance we name them (a) the smectic-planar-radial (SPR), (b) the smectic-escaped-radial (SER), (c) the chevron (CHV), (d) the bookshelf (BKS), and (e) the hybrid (HBR) structure.

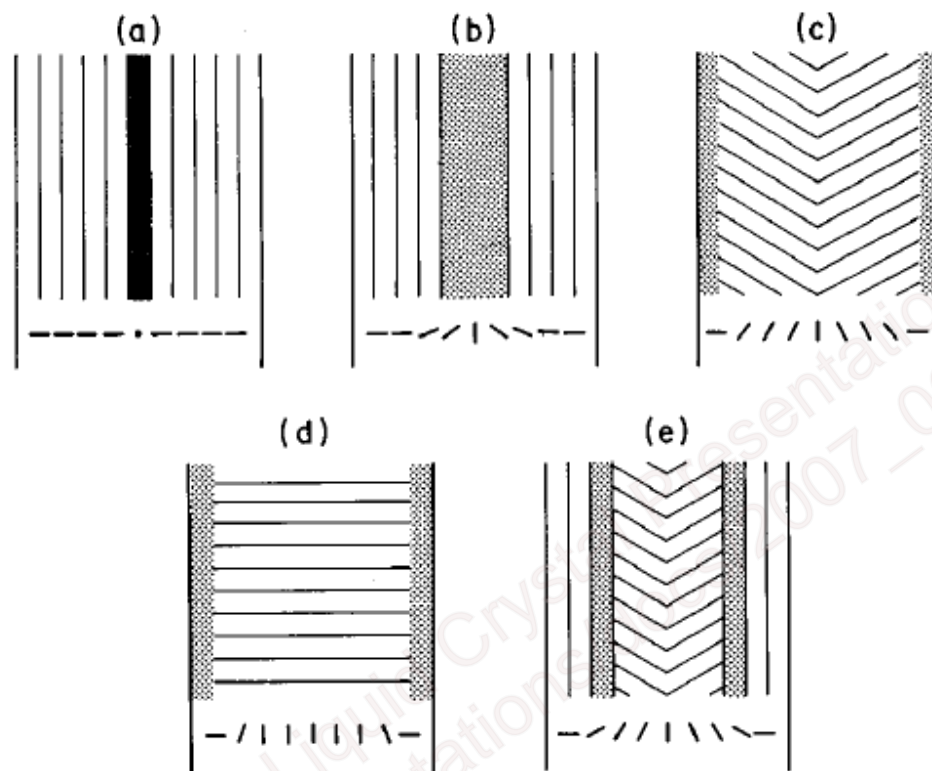


FIG. 1. Schematic presentation of different Sm-A structures for the case of strong homeotropic anchoring and smooth surface: (a) SPR, (b) SER, (c) CHV, (d) BKS, and (e) HBR structure. The smectic layers are drawn with the full line. The nematic director field spatial variation is indicated at the bottom part of each structure. The dotted regions describe places where nematic (a) or smectic (a)–(e) ordering melts.

Surface depinning of smectic-A edge dislocations

M. Slavinec,¹ S. Kralj,^{1,2} S. Žumer,^{2,3} and T. J. Sluckin⁴

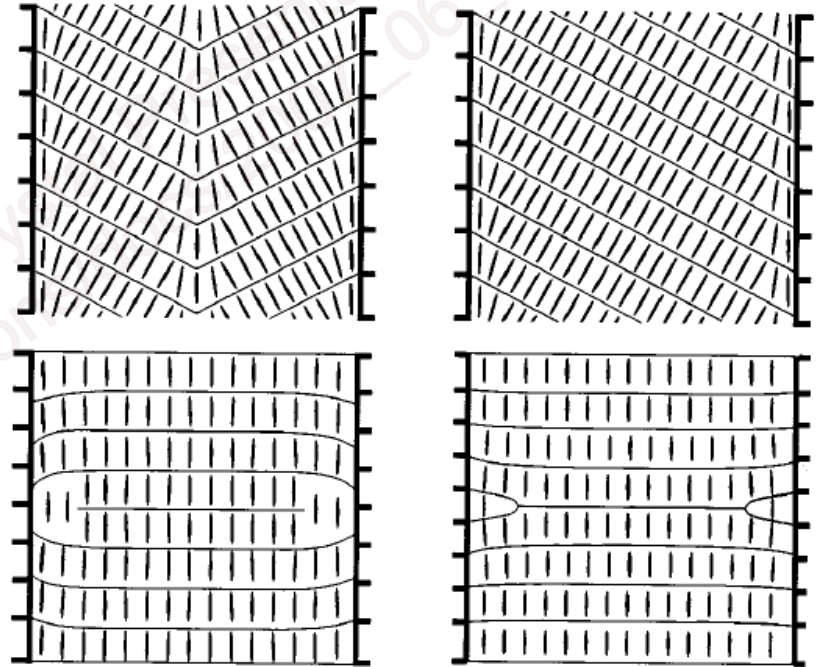
$$F = \int (f_b + f_e^{(n)} + f_e^{(s)}) d^3r + \int f_s^{(s)} d^2r,$$

$$f_b = \alpha \frac{T - T_{NA}}{T_{NA}} |\psi|^2 + \frac{\beta}{2} |\psi|^4,$$

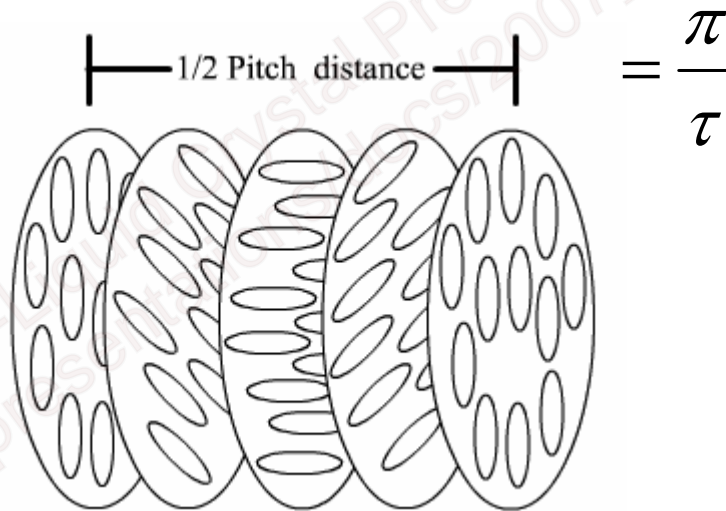
$$f_e^{(n)} = \frac{K_{11}}{2} (\nabla \cdot \mathbf{n})^2 + \frac{K_{22}}{2} (\mathbf{n} \cdot \nabla \times \mathbf{n})^2 + \frac{K_{33}}{2} (\mathbf{n} \times \nabla \times \mathbf{n})^2$$

$$f_e^{(s)} = \gamma_{\parallel} |(\mathbf{n} \cdot \nabla - iq_b)\psi|^2 + \gamma_{\perp} |(\mathbf{n} \times \nabla)\psi|^2,$$

$$f_s^{(s)} = \frac{1}{2} W_p |\psi - \psi_s|^2.$$



Cholesteric Phases



*The Phase Transition between Chiral Nematic
and Smectic A* Liquid Crystals*

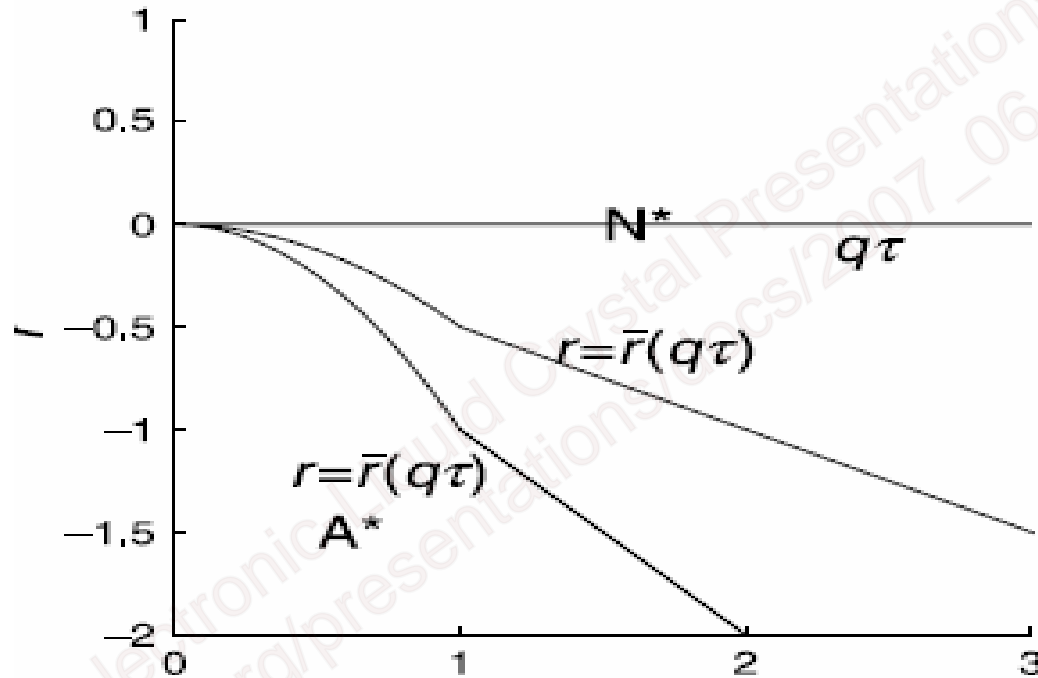
PATRICIA BAUMAN, M. CARME CALDERER, CHUN LIU,
DANIEL PHILLIPS

$$\mathfrak{F} = \int_{\Omega} [F_A + F_N] d\mathbf{x},$$

$$F_N = K_1(\nabla \cdot \mathbf{n})^2 + K_2(\mathbf{n} \cdot \nabla \times \mathbf{n} + \tau)^2 + K_3|\mathbf{n} \times (\nabla \times \mathbf{n})|^2 \\ + (K_2 + K_4)(\text{tr}(\nabla \mathbf{n})^2 - (\nabla \cdot \mathbf{n})^2).$$

$$F_A = |(i\nabla + q\mathbf{n})\Psi|^2 + r|\Psi|^2 + \frac{g}{2}|\Psi|^4.$$

Chirality introduces a stress onto the liquid crystal that affects its phase transition.



τ lowers the transition temperature

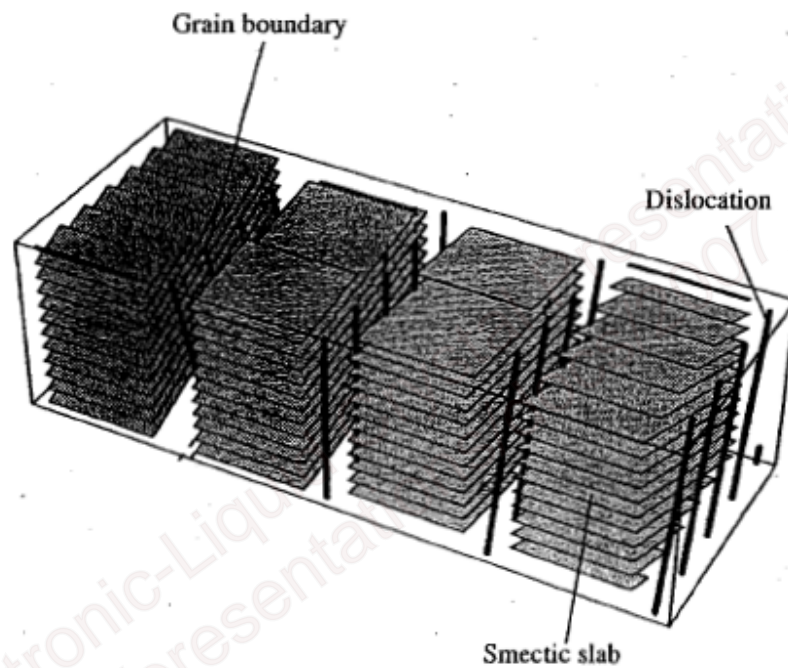
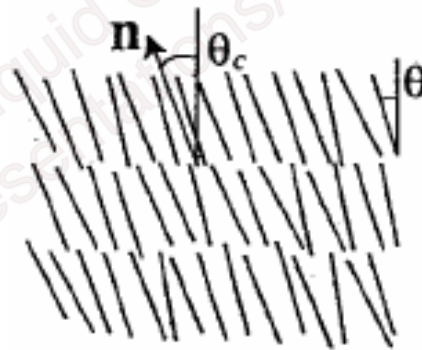


Figure 4. The structure of the smectic A TGB phase. Chirality in the material leads to a periodic melting of the smectic layers, where screw dislocations form. This results in a structure that allows the smectic layers to rotate around a helical axis.

Smectic C

$$F_{Sm} = D(\mathbb{D}^2\psi)(\mathbb{D}^2\psi)^* + [C_{||}n_in_j + C_{\perp}(\delta_{ij} - n_in_j)](\mathbb{D}_i\psi)(\mathbb{D}_j\psi)^* + r|\psi|^2 + \frac{g}{2}|\psi|^4.$$

with $\mathbb{D} \equiv \nabla - iq\mathbf{n}$,



Set $\psi = e^{i\omega(x)}$

Then

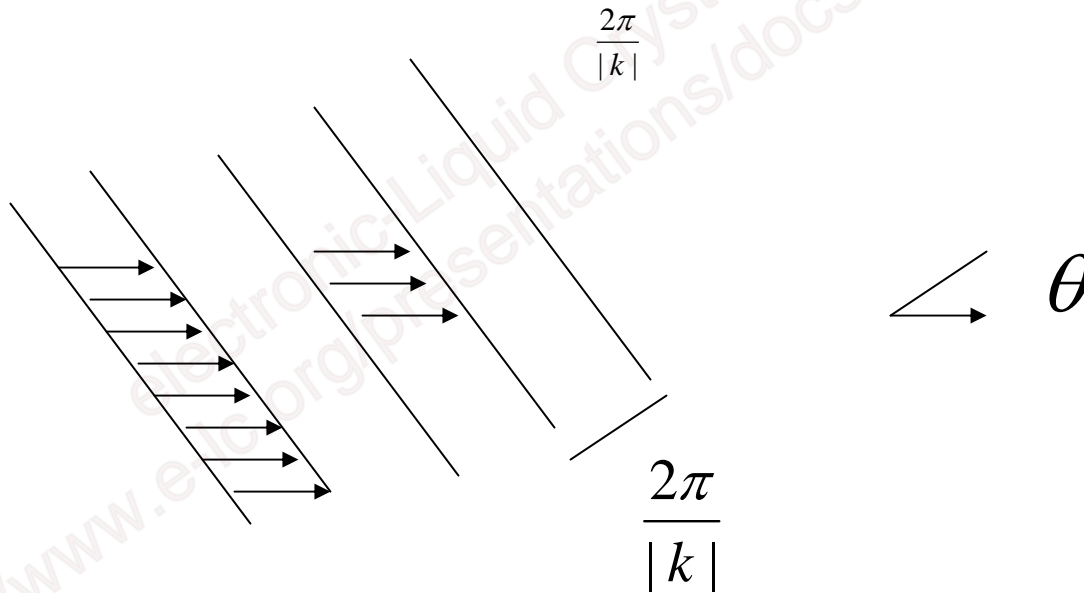
$$F_{Sm} = D(\Delta\omega - q\nabla \cdot \mathbf{n})^2 + D\left(|\nabla\omega - q\mathbf{n}|^2 + \frac{C_{\perp}}{2D}\right)^2 + C_a(\nabla\omega \cdot \mathbf{n} - q)^2 + \left(r_n + \frac{g}{2} - \frac{C_{\perp}^2}{4D}\right).$$

Now let $\omega = \mathbf{k} \cdot \mathbf{x}$ and let $\mathbf{n} = \text{const}$, then

$$F_{Sm} = D\left(|\mathbf{k} - q\mathbf{n}|^2 + \frac{C_{\perp}}{2D}\right)^2 + C_a(\mathbf{k} \cdot \mathbf{n} - q)^2 + \left(r + \frac{g}{2} - \frac{C_{\perp}^2}{4D}\right)$$

This minimizes for $|k|^2 = q^2 + \frac{|C_{\perp}|}{2D}$,

and $\cos \theta = \frac{k \cdot n}{|k|} = \frac{1}{\sqrt{1 + \frac{|C_{\perp}|}{2Dq^2}}}$



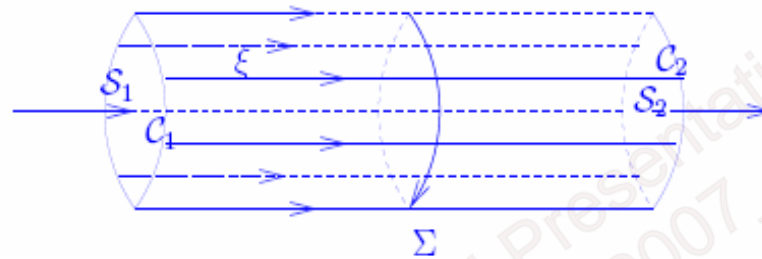
$$F_{Sm} = D(\Delta\omega - q\nabla \cdot \mathbf{n})^2 + D\left(|\nabla\omega - q\mathbf{n}|^2 + \frac{C_{\perp}}{2D}\right)^2 + C_a(\nabla\omega \cdot \mathbf{n} - q)^2 + \left(r + \frac{g}{2} - \frac{C_{\perp}^2}{4D}\right).$$

$$F_F(\mathbf{n}) = [K_1(\nabla \cdot \mathbf{n})^2 + K_2(\mathbf{n} \cdot \nabla \times \mathbf{n})^2 + K_3|\mathbf{n} \times \nabla \times \mathbf{n}|^2 + (K_2 + K_4)[\text{tr}(\nabla\mathbf{n})^2 - (\nabla \cdot \mathbf{n})^2]]$$

$$F = \int_{\Sigma} (F_{Sm} + F_F) dx$$

Boundary value problem for F.

M. Calderer and J.Park



$$\begin{cases} \nabla\omega \cdot \nu = 0 \text{ on } \Sigma, & \nabla\omega \cdot \nu_i = k \text{ on } S_i, \quad i = 1, 2, \\ |\nabla\omega|^2 = k^2 \text{ on } \Sigma \cup S_1 \cup S_2, \end{cases}$$

$$\begin{cases} \nabla\omega \cdot \nu = \pm k \text{ on } \Sigma, & \nabla\omega \cdot \nu_i = 0 \text{ on } S_i, \quad i = 1, 2, \\ |\nabla\omega|^2 = k^2 \text{ on } \Sigma \cup S_1 \cup S_2. \end{cases}$$

Such relations correspond to smectic layers reaching the boundary in a perpendicular and tangential fashion, respectively, with a prescribed wave number k .

Polarization-Modulated Smectic Liquid Crystal Phases

N. Clark et al

Jakli et al

Bauman et al

