Orientation and Defect Dynamics of Sheared Lamellar Phases

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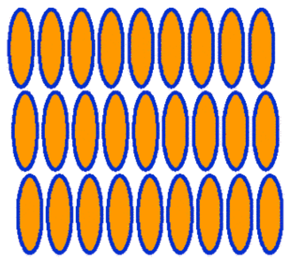
Outlines

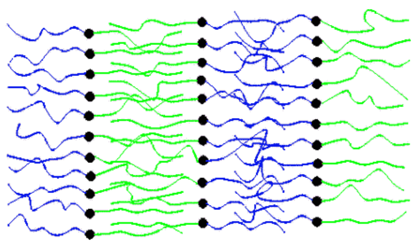
1. Introduction
2. Selection of orientations by layer instability
3. Layer orientation by dislocations
4. Defect loop model for rheology data

Lamellar Phases

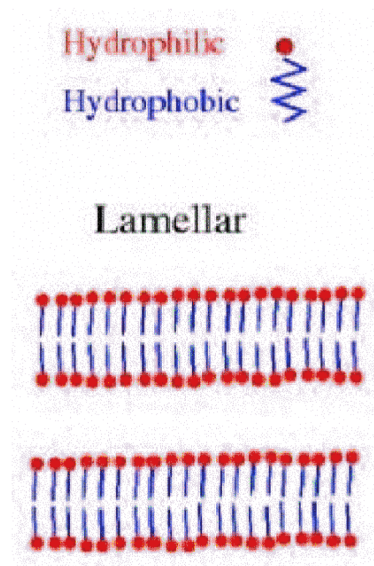
Smectic liquid crystal



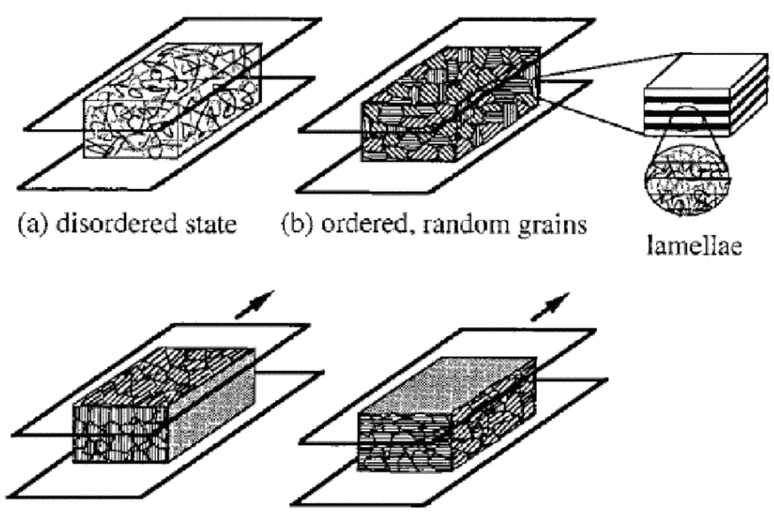
Diblock copolymer



Surfactant

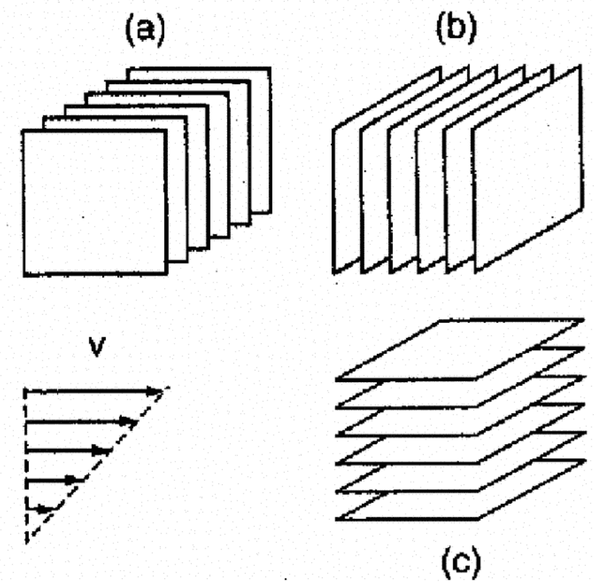


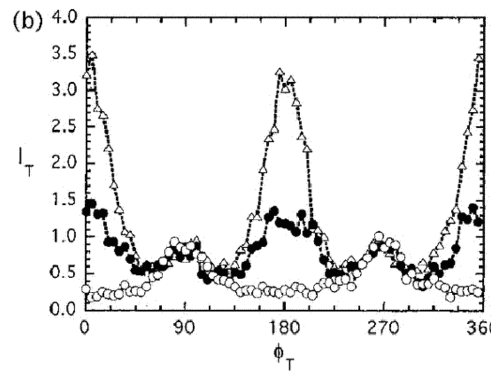
Quenched Lamellar Phases



(a) disordered state (b) ordered, random grains (c) perpendicular grains (d) parallel grains

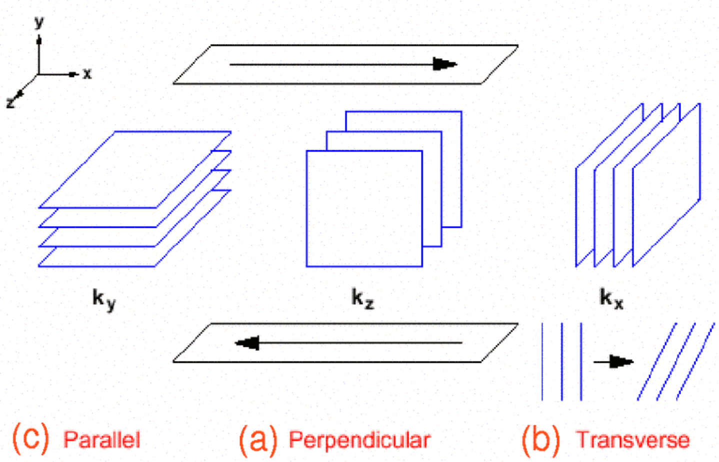
Orientations





Wang et. al. 1997

Shear Convection of Wavevector



Wavevector k convected by the shear flow as

$$k^2 \rightarrow k_x^2 + (k_y + \gamma k_x)^2 + k_z^2$$

with $\gamma =$ shear amplitude.

Shear Suppression of Fluctuation

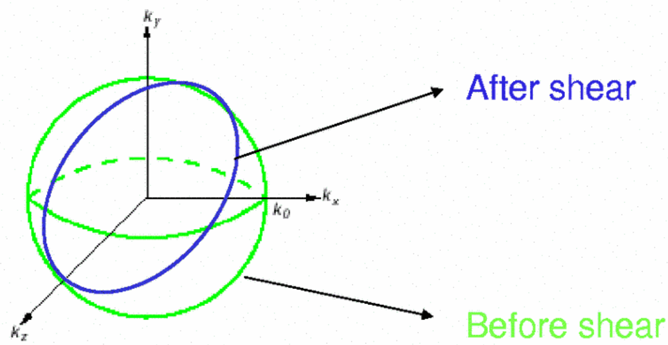
The Landau-Ginzburg Hamiltonian — Cates & Milner 1992

$$H(\phi) = \sum_{\mathbf{k}} \left[\tau + (k - k_0)^2\right] \phi(\mathbf{k})\phi(-\mathbf{k}) + \mathcal{O}(\phi^4)$$

The two-point correlation function

$$\xi(\mathbf{k}) \equiv \langle \phi(\mathbf{k})\phi(-\mathbf{k}) \rangle \approx 1/[\tau + (k - k_0)^2]$$

ξ diverges at $\tau = 0$ and $k = k_0$ due the degeneracy of the lamellar orientations.



Shear Suppression of Fluctuation (2)

In this case $\xi(\mathbf{k})$ at $k_x \ll k_0$ becomes

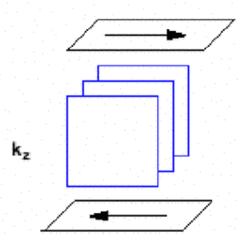
$$\xi(\mathbf{k}) = \mu \int_0^\infty dt \exp\left\{-\mu \int_0^t [\tau + (k'^2 - k_0)^2]\right\}$$
$$k'^2 = k_y^2 + k_z^2 + 2\gamma k_x k_y$$

Then as $\tau \to 0$, it can be shown that

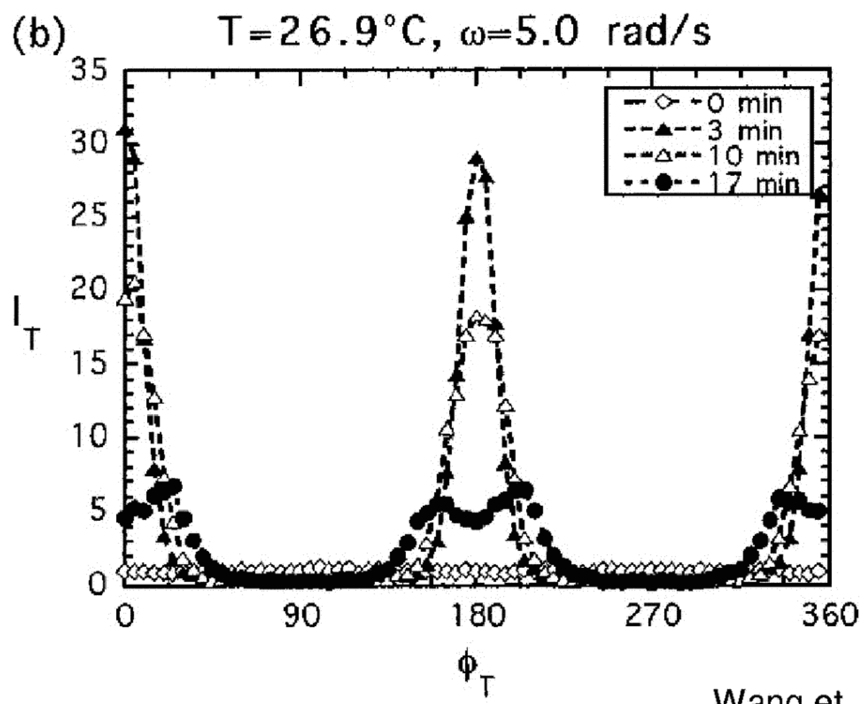
$$\mu\left\{\tau + b\gamma k_x k_y + c(\gamma k_x)^2\right\}\xi \approx 1$$

So the divergence of $\xi(k_x \to 0)$ will be largest with $k_y = 0$, leading to a wavevector

$$(0, 0, k_0) \to \text{perpendicular alignment}$$



Zigzag in Experiments



Wang et. al. 1997

Mesoscopic Dynamics

Order parameter

$$\psi(\mathbf{r}) = [\rho_A(\mathbf{r}) - \rho_B(\mathbf{r})]/2\rho_0$$

Free energy density [Leibler 1980]

$$F = \int d\mathbf{r} \left(\frac{\kappa}{2} |\nabla \psi|^2 - \frac{\tau}{2}\psi^2 + \frac{u}{4}\psi^4 \right) + \frac{B}{2} \int\int d\mathbf{r} d\mathbf{r}' G(\mathbf{r} - \mathbf{r}') \psi(\mathbf{r}) \psi(\mathbf{r}')$$

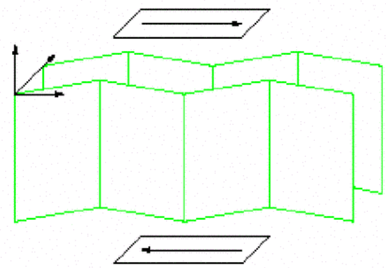
κ, τ, and B are related to N (polymerization), b (segment length) and χ (Flory-Huggins parameter) [Ohta & Kawasaki 1986].

Time-dependent Ginzburg-Landau Eq.

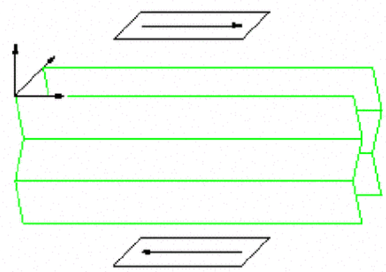
$$\frac{\partial \psi}{\partial t} + (\mathbf{v} \cdot \nabla)\psi = M \nabla^2 \frac{\delta F}{\delta \psi} = \nabla^2 \left(-\psi + \psi^3 - \nabla^2 \psi \right) - B\psi$$

Zigzag for a-Orientation

Zigzag in transverse direction : $q \uparrow$

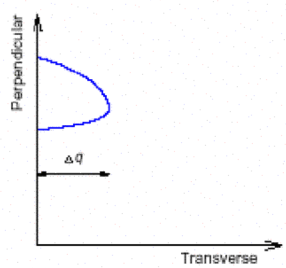


Zigzag in parellel direction : $q \cdot$



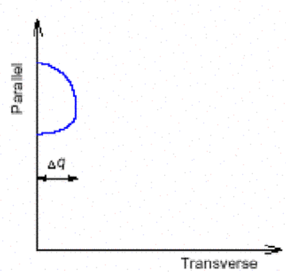
Stability Diagram in q Space

Almost Perpendicular State



$$q = \left[\Delta q^2 + q_0^2 + (a\Delta q)^2\right]^{\frac{1}{2}}$$
$$\approx q_0\left[1 + \frac{1}{2}(1+a^2)\left(\frac{\Delta q}{q_0}\right)^2\right]$$
$$\Rightarrow \left(\frac{\Delta q}{q_0}\right)^2 \leq \delta$$

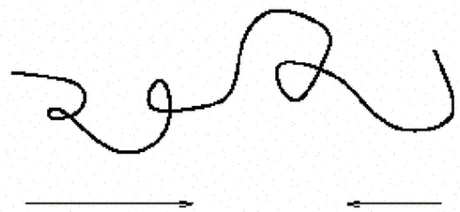
Almost Parallel State



$$q = \left[\Delta q^2 + (a\Delta q + q_0)^2\right]^{\frac{1}{2}}$$
$$\approx q_0\left(1 + a\frac{\Delta q}{q_0}\right)$$
$$\Rightarrow \frac{\Delta q}{q_0} \leq \delta$$

Chen & Vinals 2002

Where is Polymer? - Stress Coupled Dynamics



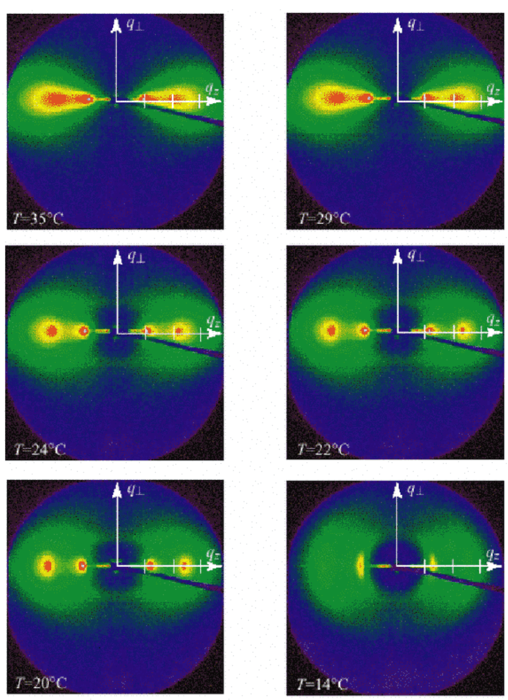
Build a model with one scalar $\psi(\boldsymbol{r}, t)$, one vector $\boldsymbol{u}(\boldsymbol{r}, t)$, and one tensor $\boldsymbol{\sigma}(\boldsymbol{r}, t)$,

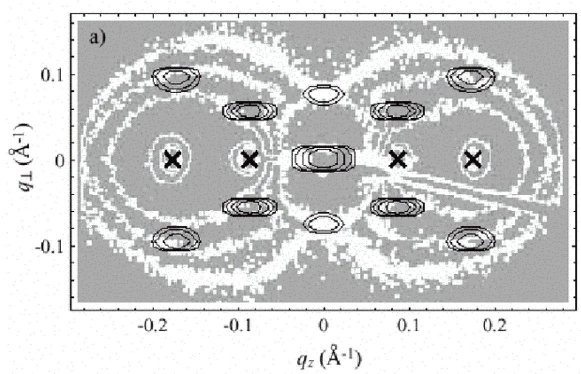
$$\frac{\partial \psi}{\partial t} + (\boldsymbol{u} \cdot \boldsymbol{\nabla})\psi = M\left(\nabla^2 \frac{\delta F}{\delta \psi} - \alpha \boldsymbol{\nabla}\boldsymbol{\nabla} : \boldsymbol{\sigma}_p\right)$$

Helfand & Fredrickson

Screw Defect in Smectic

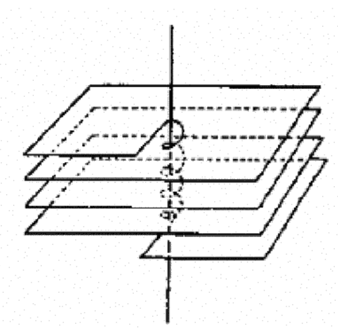
Lamellar phase of C12E5/DMPC-water



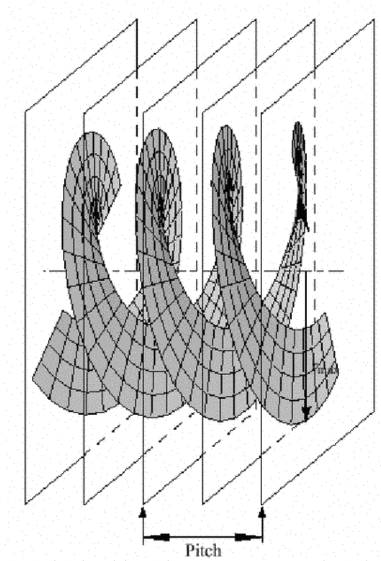


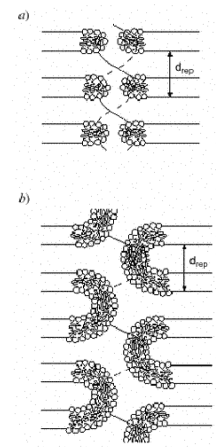
Dhez et. al. 2000

Screw Dislocations



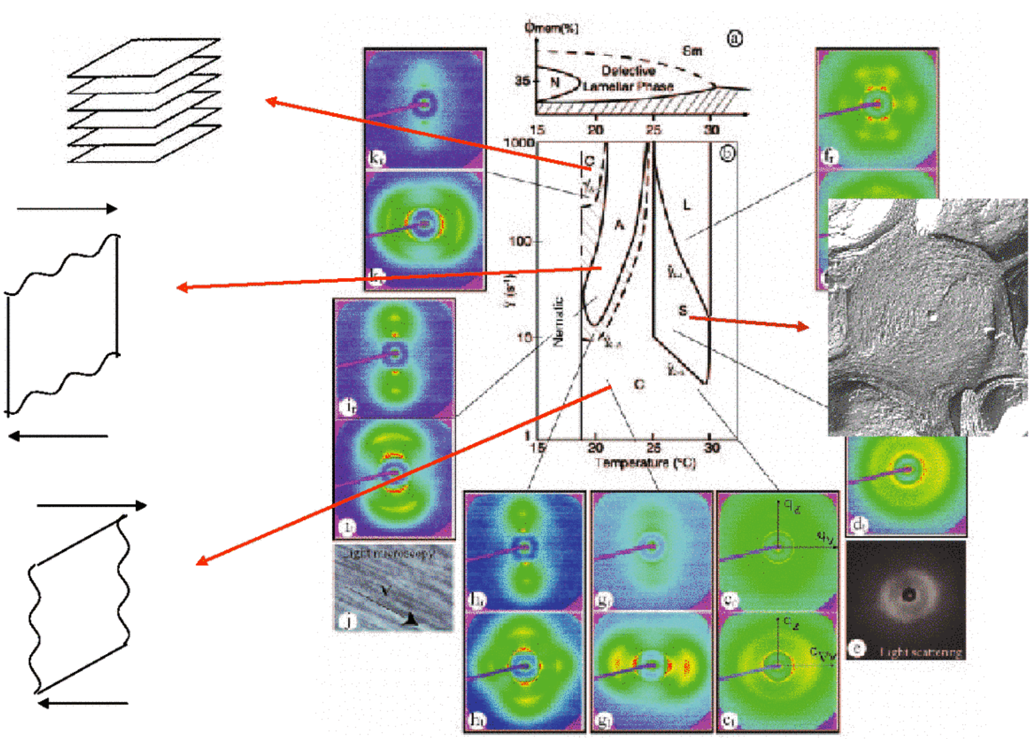
A simple screw dislocation





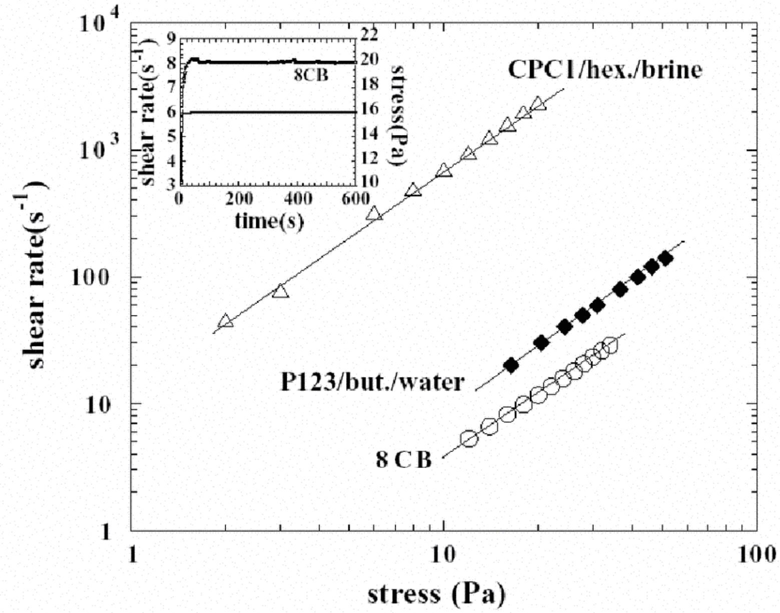
Twin helices → Burgers vector 2

Influence of Screw on Orientation



Dhez et. al. 2001

Steady Shear Rheology Data

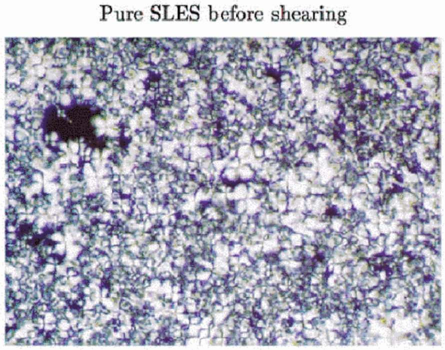


- **Very viscous**
- **Shear thinning**

Meyer, Asnacios, Kleman, 2001

Transient study:Less defects, Less viscous

Pure SLES before shearing



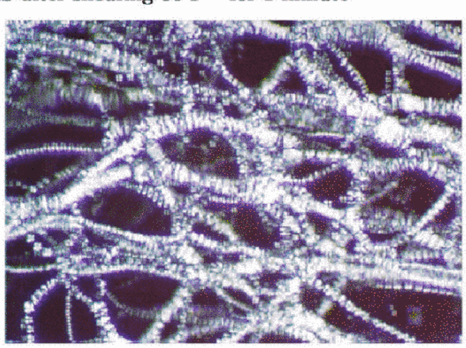
Basappa et. al. 1999

Sodium dodecyl ether sulphate (SLES) + Water

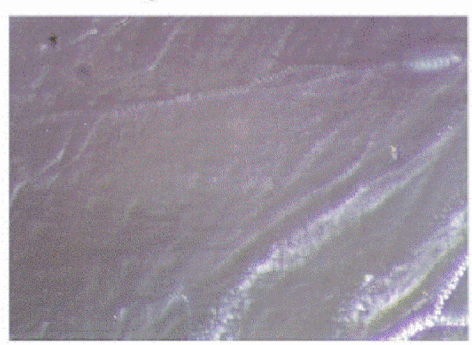
$$CH_3 - (CH_2)_{10} - [OC_2H_4] - SO_4^- Na^+$$

$$\text{SLES} : H_2O = 72.3:26.8$$

Pure SLES after shearing 58 s^{-1} for 1 minute



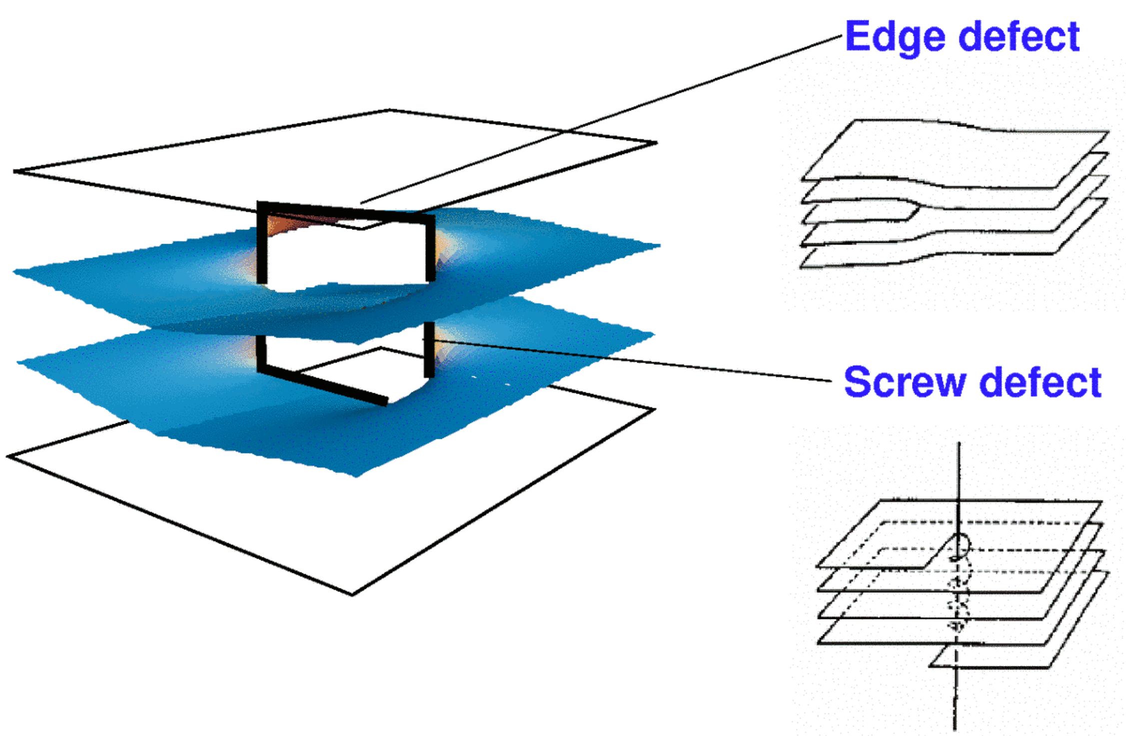
Pure SLES after shearing 58 s^{-1} for 13 minute



Existing Theories for Smectic Viscosities

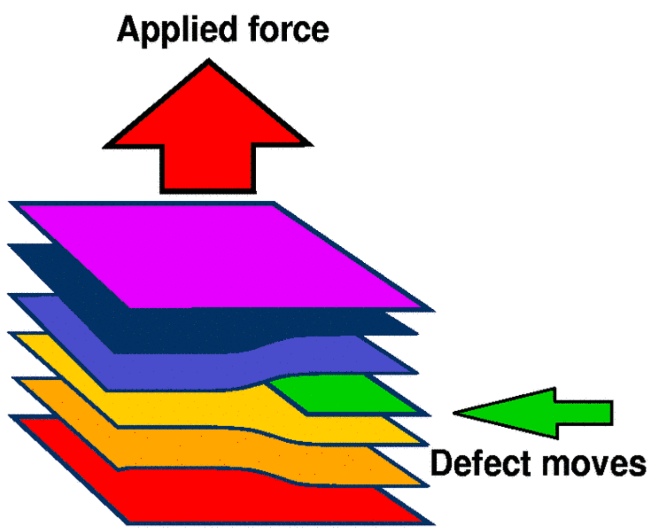
- Fluctuations
  (Mazenko, Ramaswamy, and Toner, 1982, Milner 1986)
- Textures (Kawasaki, Onuki 1990)
- Defects (Meyer, Asnacios, Klemen 2001)

We consider the defect loops in smectics

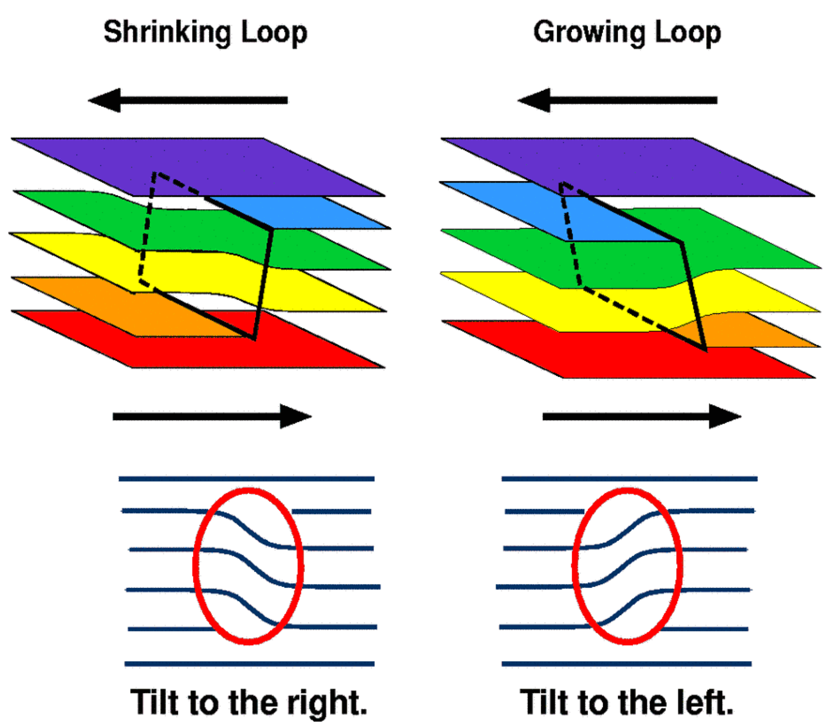


Peach-Koehler force on defect lines

Stress driven defect motion $f = \tau \times (\sigma \cdot \mathrm{n} b)$

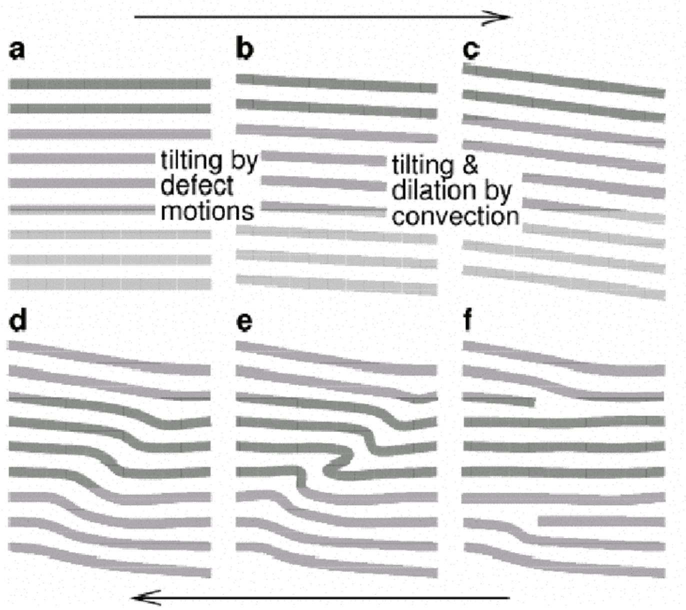


Peach-Koehler Force Acting on Defect Loops

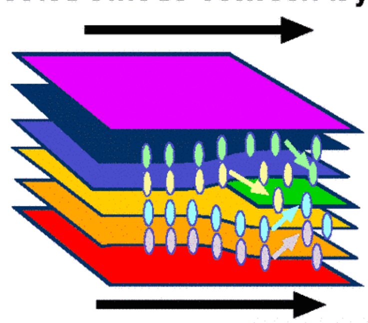


Undulation Instability under Flow

Effects of the instability: (1) Produce more defects.
(2) Tilt the layers backward.



Stress from Permeation



Oswald & Allain

- Flow through the defect $\sim l_s\dot{\gamma}$
- The viscous force $\sim l_e\frac{(l_s\dot{\gamma})}{\mu}$
- Dissipation per unit volume

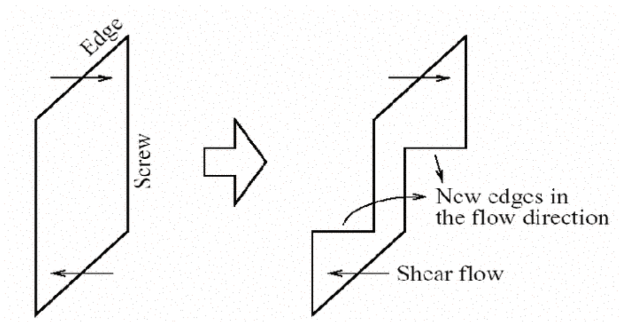
$$T\dot{s} \simeq n_0 l_e \frac{(l_s\dot{\gamma})^2}{\mu} = \underbrace{\left(n_0 l_e \frac{l_s^2}{\mu}\dot{\gamma}\right)}_{\text{stress}}\dot{\gamma}$$

n_0: the number of loop per unit volume

From big loops to smaller ones

Viscous tensions : $F_s = l_e \frac{l_s \dot{\gamma}}{\mu}$

- If $F_s > \Gamma_e$, the edge energy, new edges will be produced.
- The elongated loops have more chances to collide with the other loops.



Therefore

$$l_e \frac{l_s \dot{\gamma}}{\mu} \simeq \Gamma_e$$

Screw Density

$$\partial_t n_F = \frac{1}{b l_e} \dot{\gamma} - \frac{\dot{\gamma} l_s}{l_\Delta} n_F$$

- Source by the instability
- Sink by the flow induced collision

$$n_F \sim \left(\frac{1}{b l_s l_e}\right)^{2/3} \sim \left(\frac{\dot{\gamma}}{b \mu \Gamma_e}\right)^{2/3}$$

Stress Scaling

Shear Thinning

$$\sigma \simeq (n_0 l_s)\left(\frac{l_s l_e}{\mu}\dot\gamma\right) \simeq n_F \Gamma_e \sim \frac{\Gamma_e^{1/3}}{(\mu b)^{3/2}}\dot\gamma^{2/3}$$

Small Burgers' vector $\Gamma_e \sim Bb^2$

$$\sigma \sim \frac{B^{1/3}}{\mu^{2/3}}\dot\gamma^{2/3}$$

Lu & Chen

Compared to Experiments

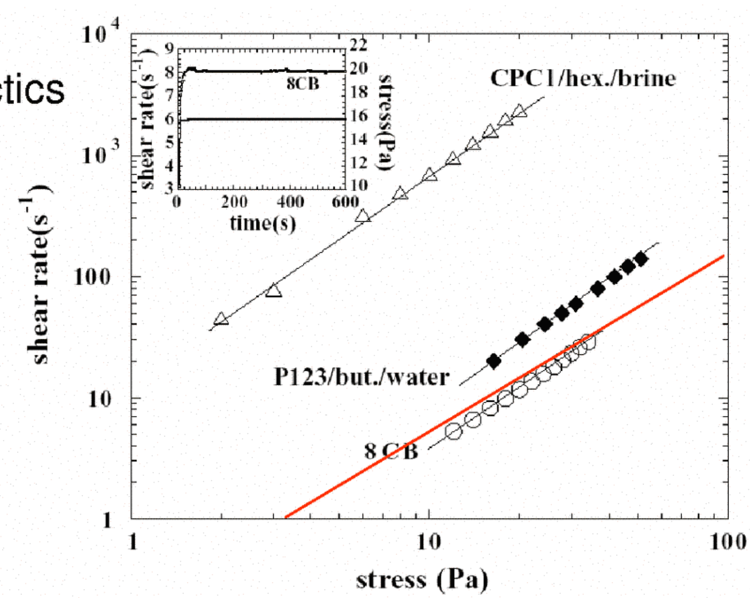
Typical thermotropic smectics

$B \sim 10^6$Pa.

$\mu_c \sim 10$cmsg^{-1}

$\dot\gamma \sim 10$sec^{-1}

Shear stress ~ 20 Pa.



Red line has the slop 3/2

Summary

- Dynamical selection of orientations
- Layer orientation by dislocations
- Defect loop model for rheology data