Simulating Shear (and More Complex) Flows of Liquid-Crystalline Polymers

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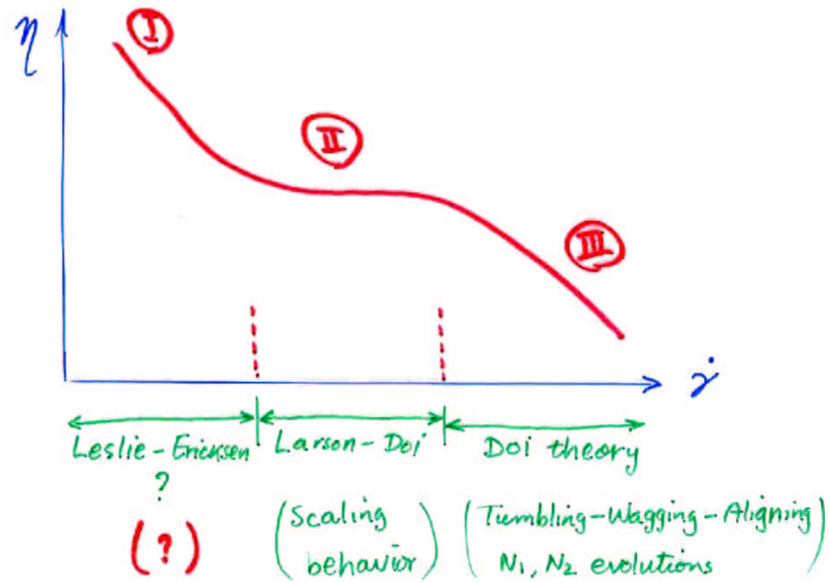

⟵ complete theory ⟶
(?)

JF:
1. Apply Leslie-Ericksen theory to sheared Monodomains, to explore the nucleation of defects.
2. Develop a "complete" constitutive theory.

GS → 3. Apply such a theory to shear flow simulations.

Previous experimental work: Larson & Mead (1993)

Increasing Shear Rate →

Stripes appear	Refinement; irregular; disclinations	Director turbulence

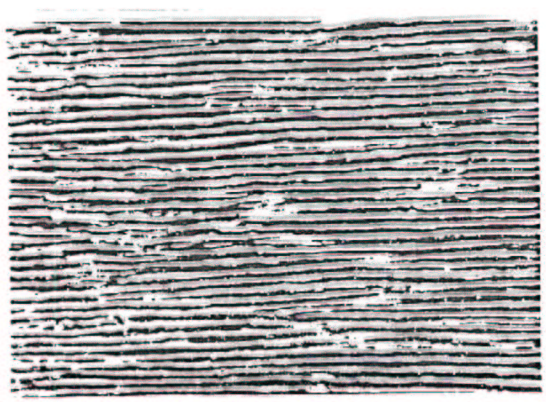

Figure 7. Thin stripes for PBG198 at a gap of $25\,\mu$ and a velocity of $3{\cdot}5\,\mu s^{-1}$ after 9 min of shearing. The sample is viewed between crossed 0°–90° polarizers, with a quarter-wave plate inserted with slow axis at 45°. $Vd = 87{\cdot}5\,\mu^2 s^{-1}$.

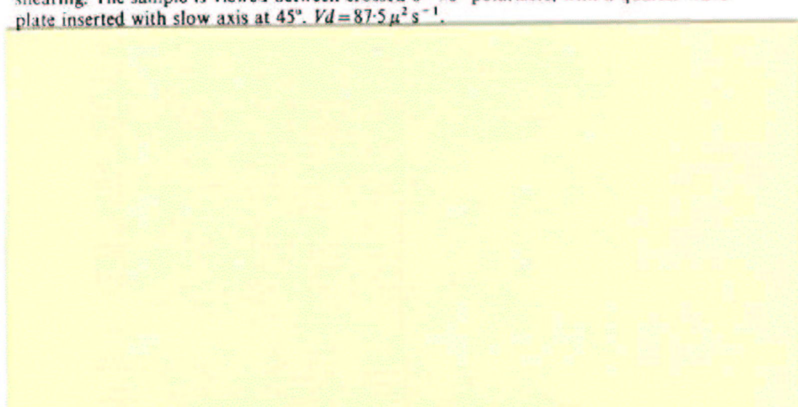

Figure 8. Irregular stripes observed for PBG198 at a gap of $50\,\mu$ and a velocity of $10\,\mu s^{-1}$ after 3 min of shearing, viewed under the same polarization conditions as figure 7. $Vd = 500\,\mu^2 s^{-1}$.

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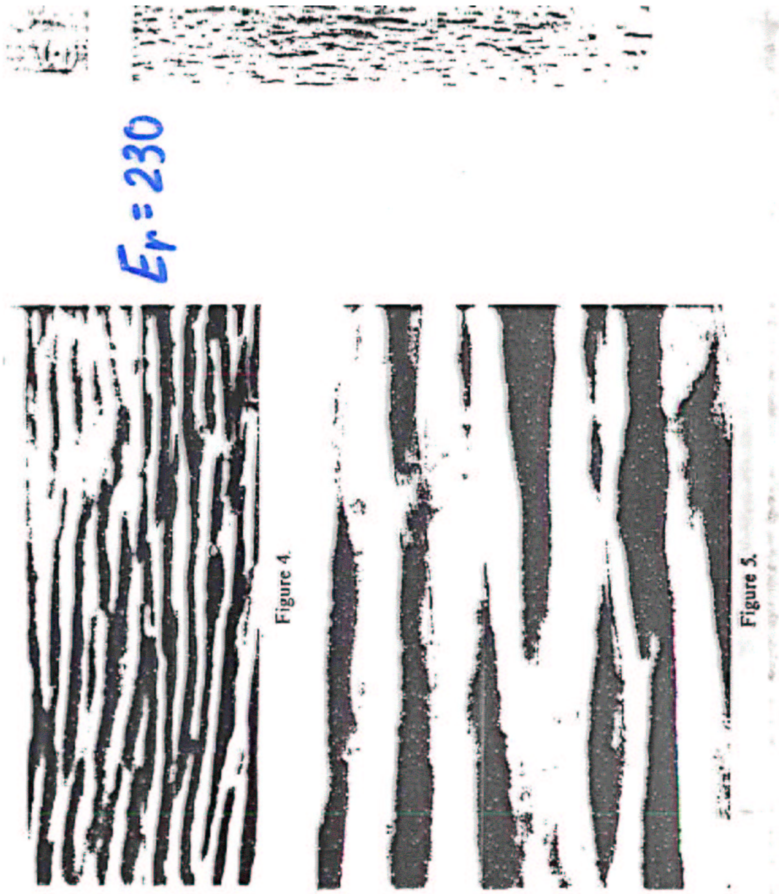


Figure 4.

Figure 5.

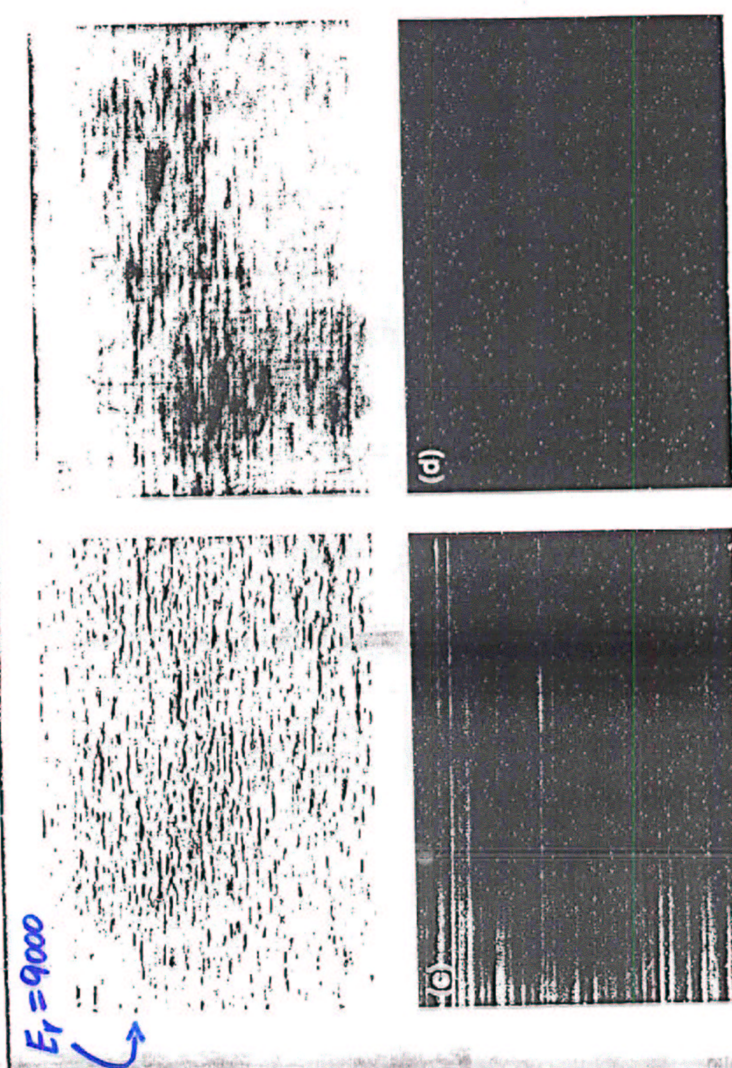


Figure 9. Texture between crossed 45°–135° polarizers, produced by shearing PBLG238 at a gap of 250 μ and shear rates $\dot{\gamma}$ of (a) 0·1, (b) 1, (c) 10 and (d) 40 s^{-1} for at least 100 strain units. Here the sample is viewed through a × 10 objective, with a field of view 0·7 mm across. Although there are no stripes in (d) at 40 s^{-1}, stripes are visible at this shear rate if the polaroids are rotated to 10°–100°. However, no stripes can be seen under any polarization conditions when $\dot{\gamma} > 75\ s^{-1}$.

?

Previous theoretical work:

- Linear instability analysis using Leslie-Ericksen theory:

  Manneville & Dubois-Violette (1976);
  Larson (1993).

Objectives of this work:

- Use direct flow simulations to follow the nonlinear evolution of roll cells;
- Explore birth of disclinations in distorted orientational fields.

The Leslie-Ericksen Theory

1. Rotation of the director: balance between viscous and elastic torque

$$\boldsymbol{n}\times(\boldsymbol{h}-\gamma_1\boldsymbol{N}-\gamma_2\boldsymbol{D}\cdot\boldsymbol{n})=\boldsymbol{0}$$

$\boldsymbol{h}$: elastic torque ⇐ free energy of elastic distortions (splay, twist, bend. K)

$\boldsymbol{N}, \boldsymbol{D}\cdot\boldsymbol{n}$: viscous torque (viscosities: γ_1, γ_2)

$$\underline{N} = \dot{\underline{n}} - \underline{\Omega}\cdot\underline{n}$$

2. Stress tensor:

$$\sigma = \sigma_e + \alpha_1\boldsymbol{D}:\boldsymbol{nnnn} + \alpha_2\boldsymbol{nN} + \alpha_3\boldsymbol{Nn} + \alpha_4\boldsymbol{D} + \alpha_5\boldsymbol{nn}\cdot\boldsymbol{D} + \alpha_6\boldsymbol{D}\cdot\boldsymbol{nn}$$

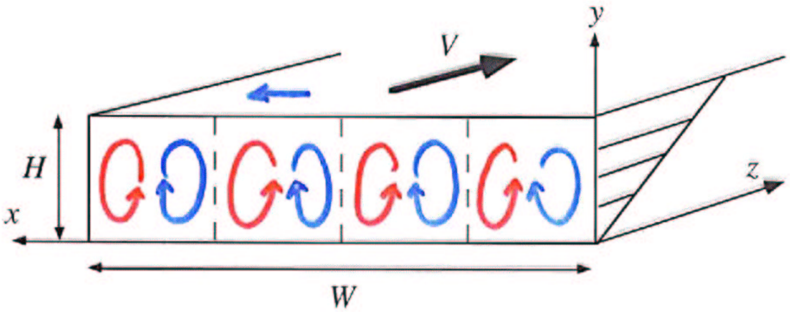
Elastic stress

3. Equations of motion:

$$\nabla\cdot v = 0, \qquad \boldsymbol{0} = -\nabla p + \nabla\cdot\sigma$$

Numerical Method:

- Finite-difference method on rectangular domain:



- Width of computational domain: W/H = ?
- Anchoring conditions on top/bottom walls
- Boundary conditions on side walls

Erickson Number:

$$E_r = \eta V H / K = \eta \dot{\gamma} H^2 / K$$

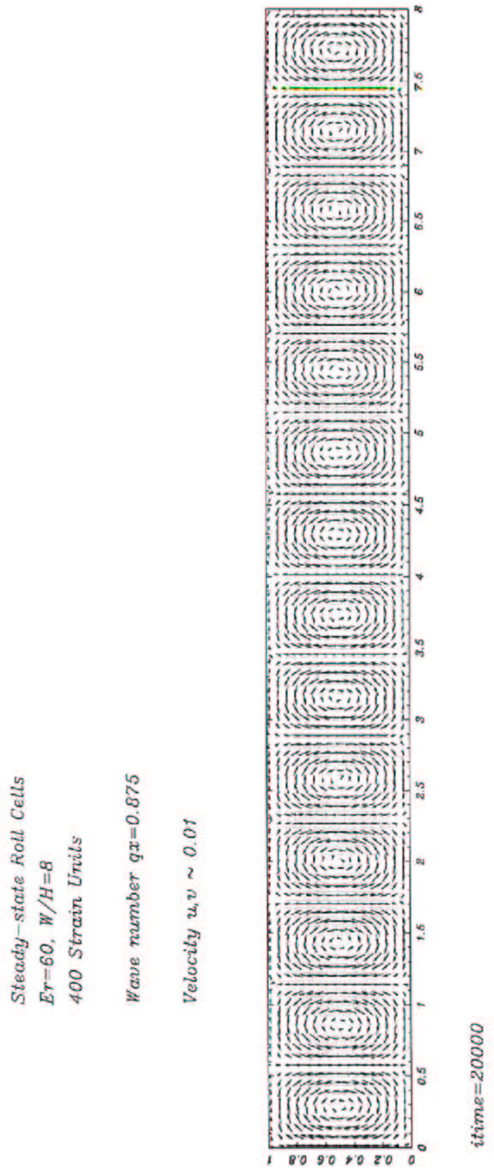
Four Regimes:

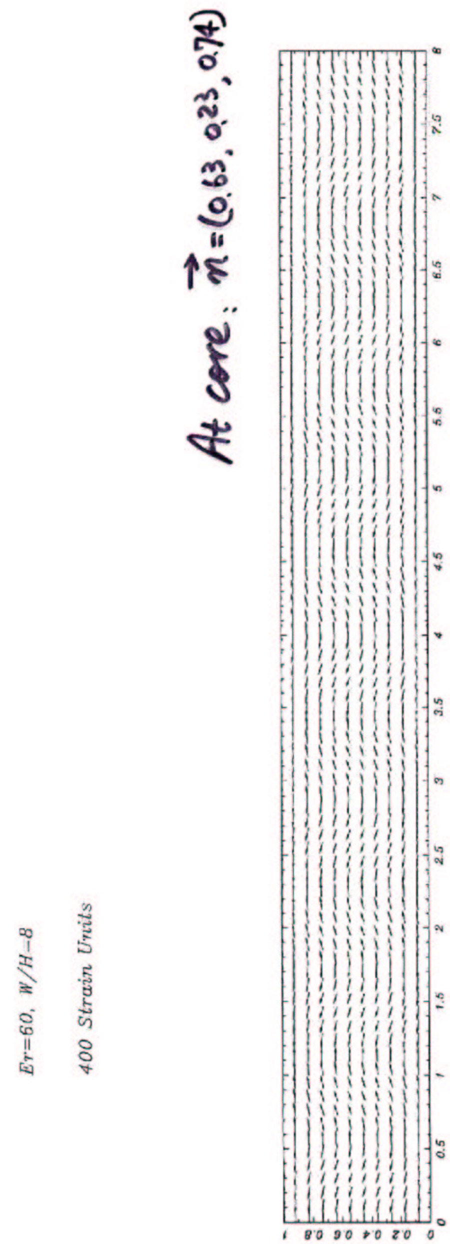
I. Stable simple shear ($0 < Er < 55$)

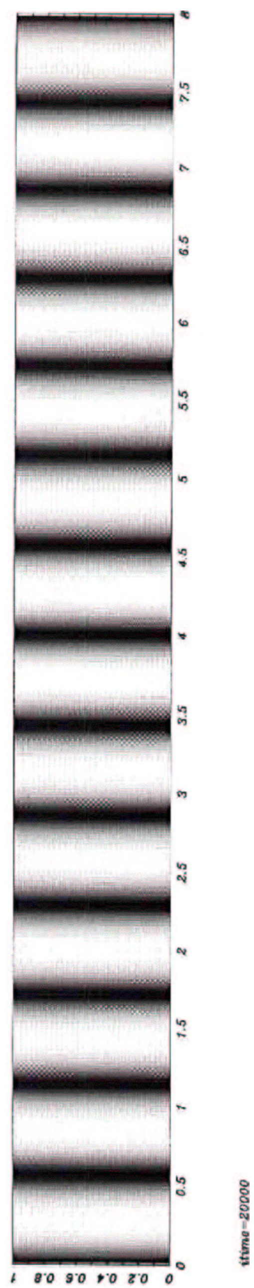
II. Steady-state roll cells ($55 < Er < 85$)

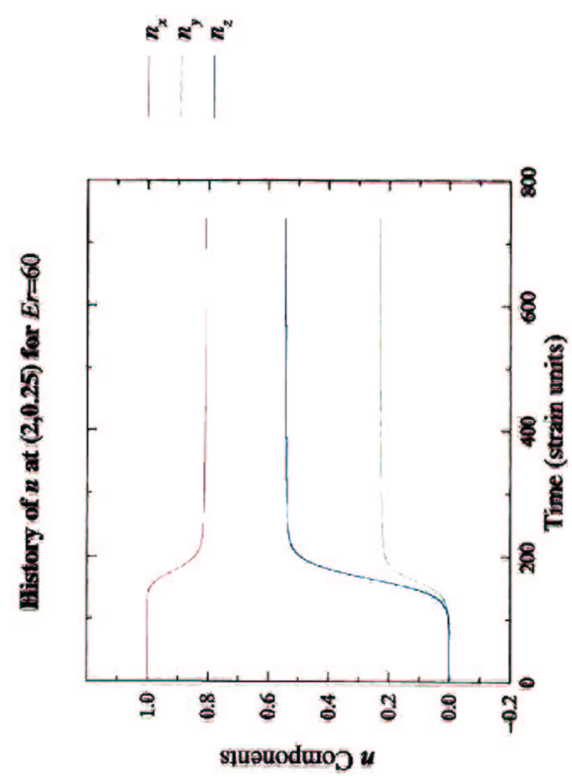
III. Oscillating roll cells ($85 < Er < 150$)

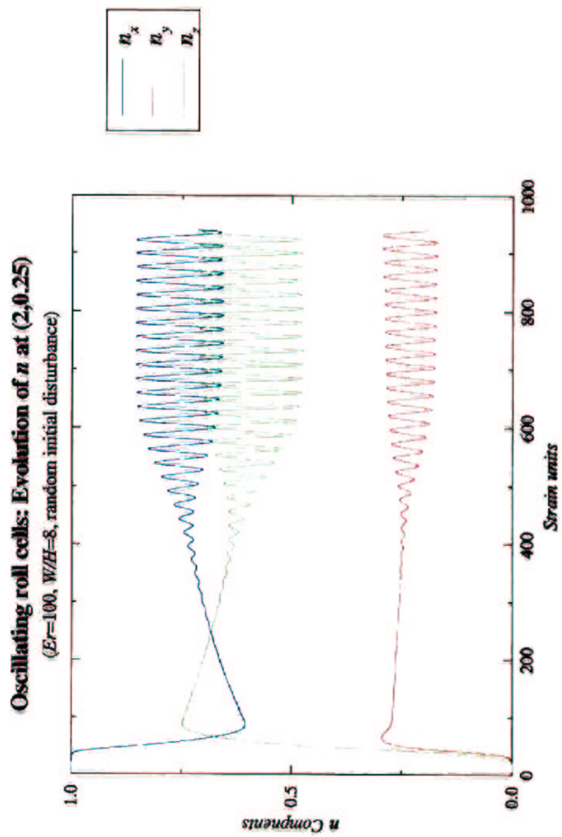
IV. Irregular patterns with defects ($Er > 150$)

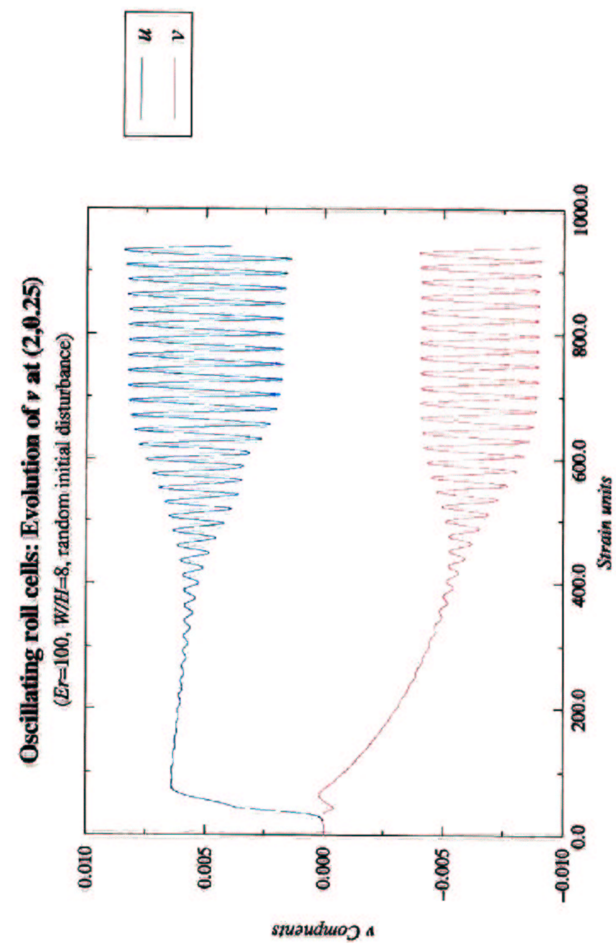

Steady-state Roll Cells
Er=60, W/H=8
400 Strain Units
Wave number qx=0.875
Velocity u,v ~ 0.01
itime=20000

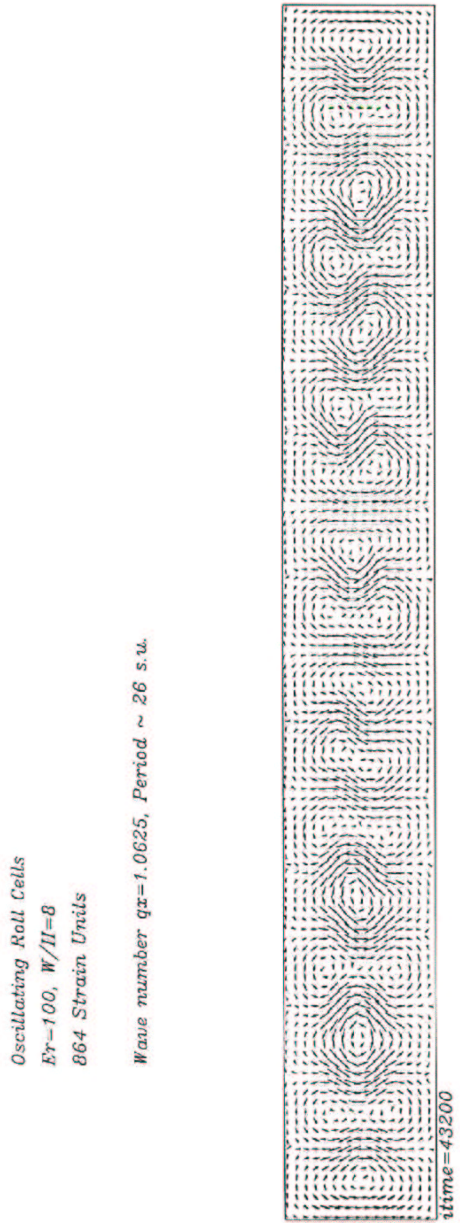

At core: $\vec{n}$ = (0.63, 0.23, 0.74)
Er=60, W/H=8
400 Strain Units


time=20000

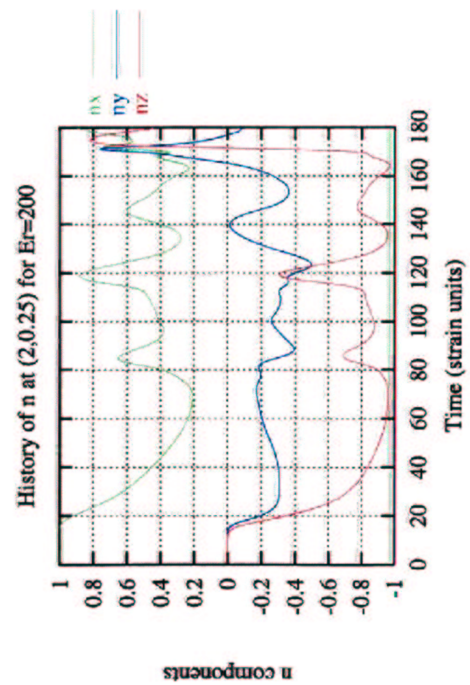

History of n at (2,0.25) for Er=60
n Components
Time (strain units)
n_x
n_y
n_z


Oscillating roll cells: Evolution of n at (2,0.25)
(Er=100, W/H=8, random initial disturbance)
n Components
Strain units
0
200
400
600
800
1000
0.0
0.5
1.0
n_x
n_y
n_z

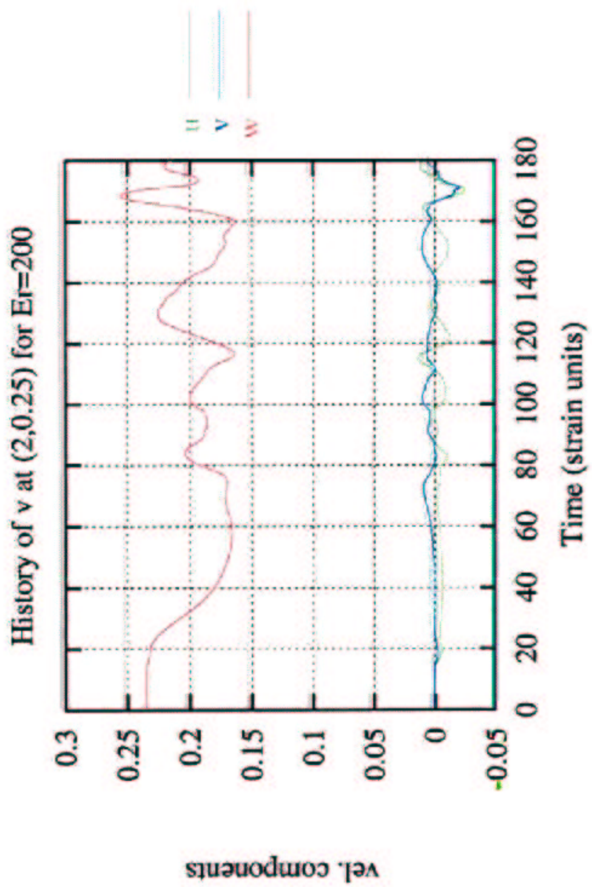

Oscillating roll cells: Evolution of v at (2,0.25)
(Er=100, W/H=8, random initial disturbance)
v Components
Strain units
0.0
200.0
400.0
600.0
800.0
1000.0
0.010
0.005
0.000
−0.005
−0.010
u
v

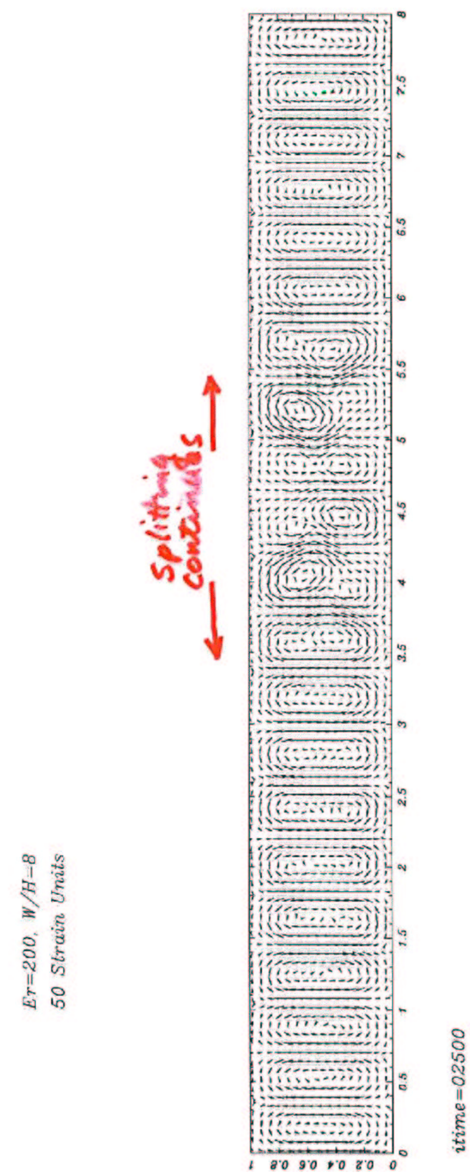

Oscillating Roll Cells
Er=100, W/H=8
864 Strain Units
Wave number qx=1.0625, Period ~ 26 s.u.
time=43200

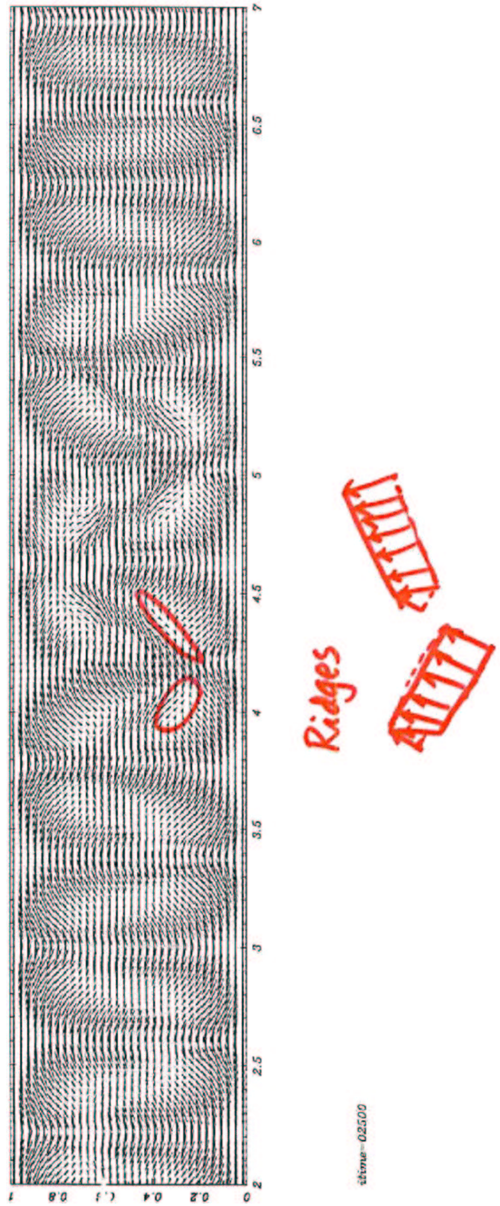
$E_r = 200$

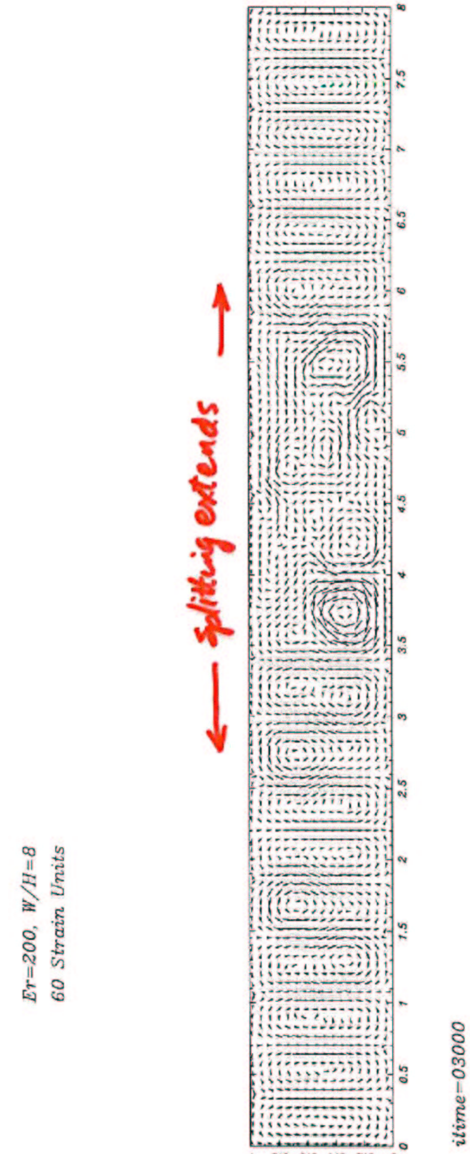

History of n at (2,0.25) for Er=200
nx
ny
nz
n components
Time (strain units)

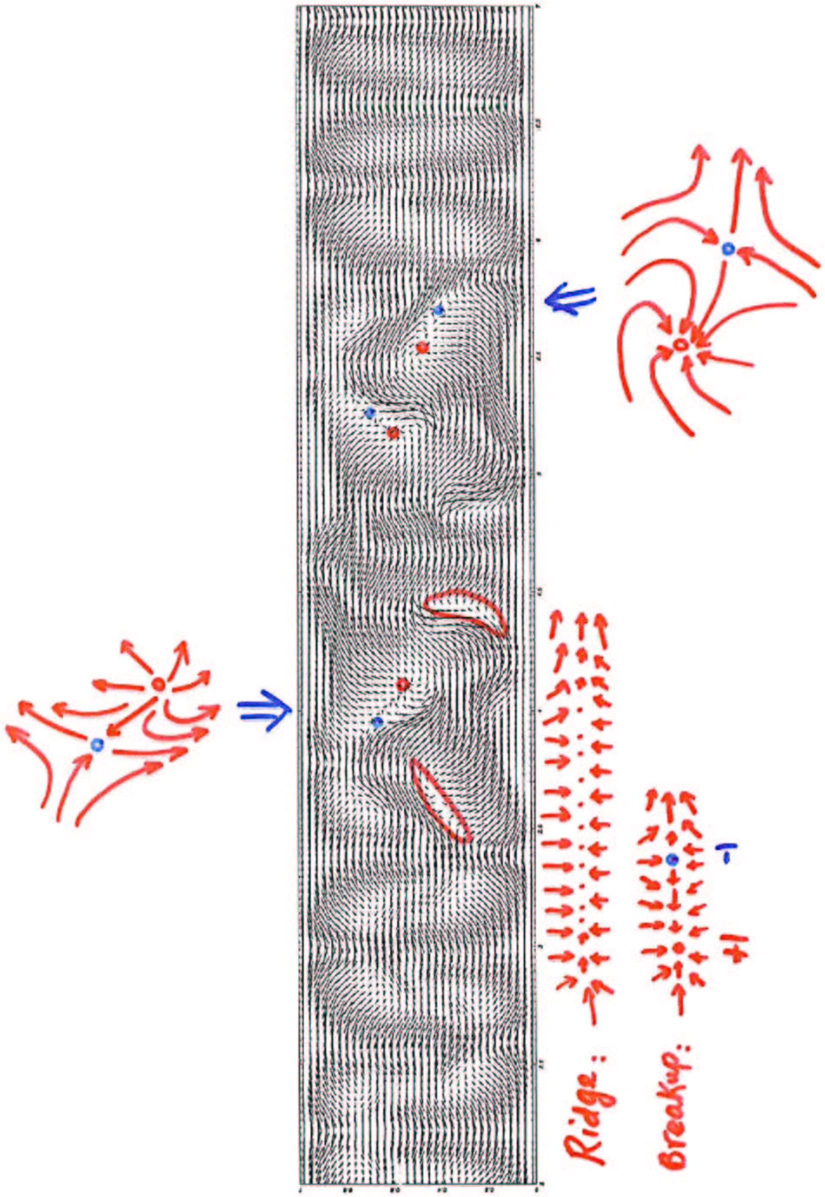
$E_r = 200$

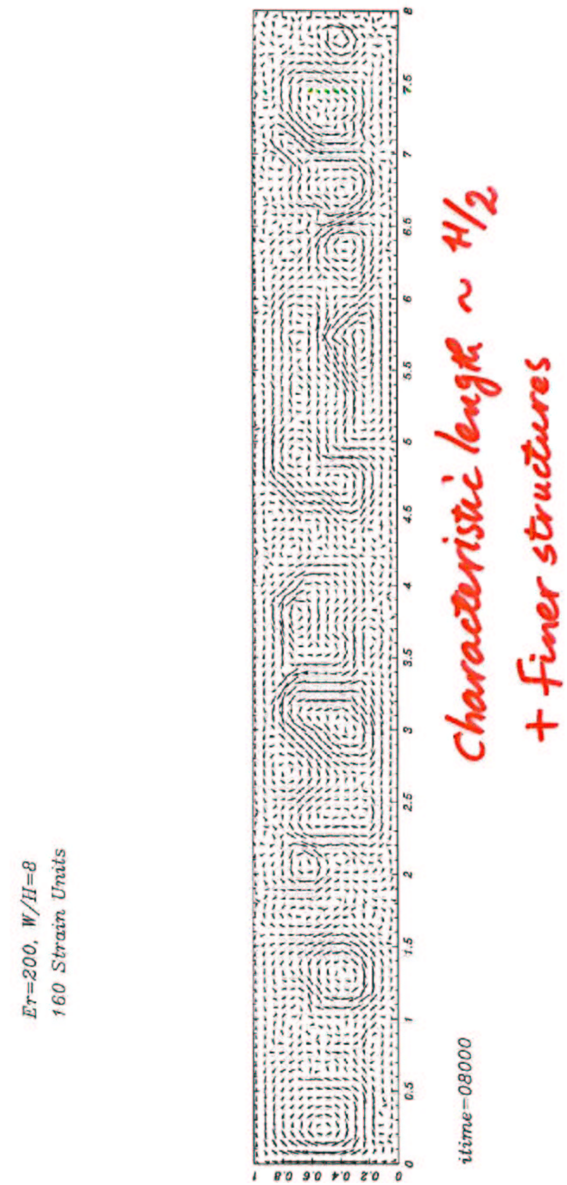

History of v at (2,0.25) for Er=200
vel. components
Time (strain units)
u
v
w
0.3
0.25
0.2
0.15
0.1
0.05
0
-0.05
0
20
40
60
80
100
120
140
160
180

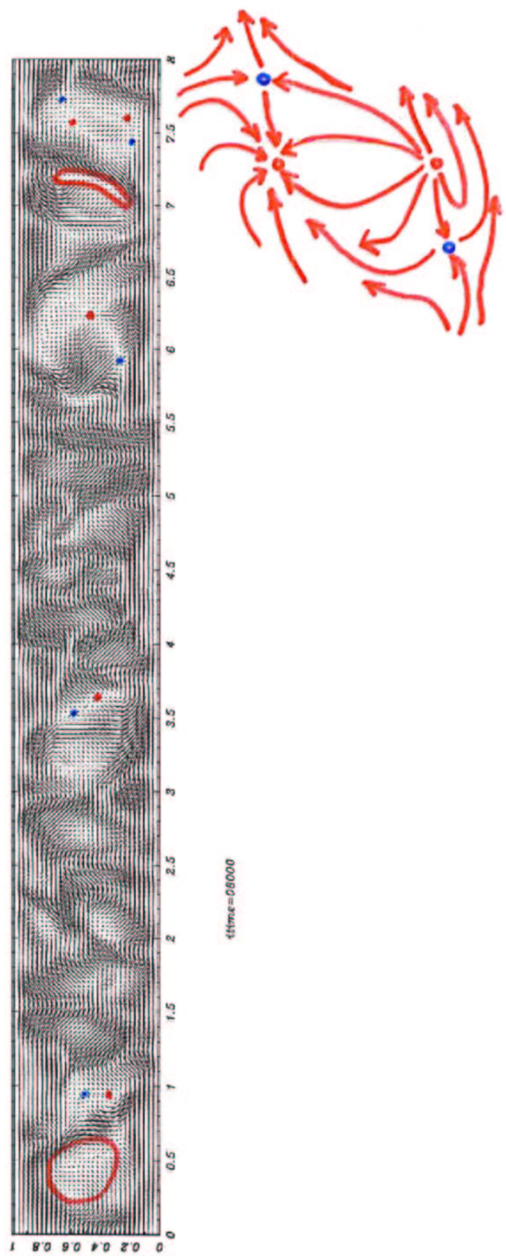

Er=200, W/H=8
50 Strain Units
itime=02500
Splitting continues


Ridges
itime=02500


splitting extends
Er=200, W/H=8
60 Strain Units
itime=03000


Ridge:
Breakup:
+1


Er=200, W/H=8
160 Strain Units
itime=08000
Characteristic length ~ H/2
+ Finer structures



Comparison with experiment (Larson & Mead 1993):

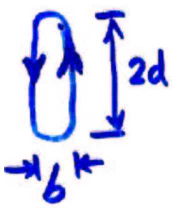
Four regimes in general agreement.

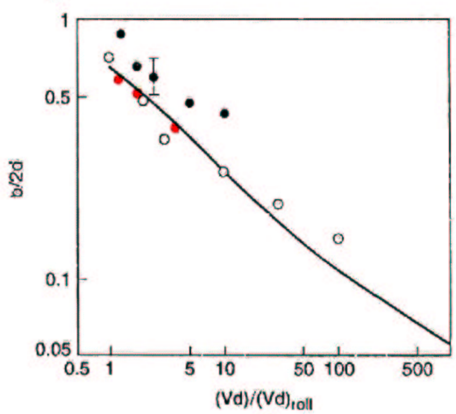
1. The appearance and growth of roll cells:
   - Onset: $Er = 55$ (numerical); $Er = 45$ (experiment);
   - Agreement of wave numbers; increase with Er.
2. Long-time behavior of roll cells at higher Er:
   - Numerical: Rolls split and oscillate for $85 < Er < 150$;
   - Experimental: "steady-state" rolls up to $Er = 155$.

1. Dominant modes don't change during nonlinear growth:

E_r	$b/2d$
= 60	= 0.57
100	0.47
200	0.38

2. Wave number ↑ with E_r; agrees with Experiment.





(b)

igure 10. (a) Stripe spacing as a function of plate velocity, V, for two different gaps, d, for

Comparison with experiment (Cont'd):

3. At still higher *Er*:

- Experimental: for $Er > 150 - 230$,
  - (a) "... a weaker fine structure appears, which disrupts the regularity of the striped pattern."
  - (b) thick disclinations first appear at $Er \approx 150$.
  - (c) "director turbulence" at still higher *Er*.
- Numerical: for $Er > 150$,
  - (a) rolls break up into irregular patterns; big swirls (size ~ $H/2$) surrounded by small ones.
  - (b) ±1 disclinations nucleating; persists for ~ 30 s.u.

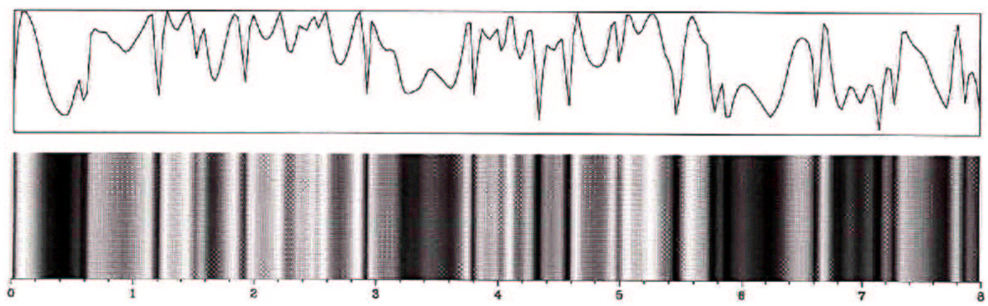


Fig. 17

Limitations

1. Dimensionality: can't represent "Director turbulence".
2. Can't reprensent ±1/2 defects.
3. Can't access Deborah-Number cascade.

⟹ the need for a "complete theory".

* Even with a complete theory, can one cover all the length scales?

A complete theory as a generalization of Doi theory.

⇒ Maier-Saupe potential:

$$U_{MS}(\underline{u}) = -\frac{3}{2} U kT \langle \underline{u}'\underline{u}' \rangle : \underline{u}\underline{u}$$

⇒ Marrucci-Greco potential:

$$U_{MG}(\underline{u}) = -\frac{3}{2} U kT \left[\langle \underline{u}'\underline{u}' \rangle + \frac{\mathcal{L}^2}{24} \nabla^2 \langle \underline{u}'\underline{u}' \rangle \right] : \underline{u}\underline{u}$$

↓ weak distortion

Frank elasticity $f = \frac{\nu kT}{6} U S^2 \mathcal{L}^2 (\nabla \underline{n} : \nabla \underline{n}^T)$

The "complete" theory has 2 parts:

1. Evolution equation for $\underline{\underline{A}} = \langle \underline{u}\underline{u} \rangle$:

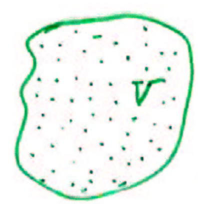
$$\frac{\partial A}{\partial t} + v \cdot \nabla A - \kappa \cdot A - A \cdot \kappa^T = -2\kappa : \langle uuuu \rangle - 6\bar{D}_r\left(A - \frac{\delta}{3}\right) + 6\bar{D}_r U (A \cdot A - A : \langle uuuu \rangle) + \frac{\bar{D}_r U \mathcal{L}^2}{8}\left[\nabla^2 A \cdot A + A \cdot \nabla^2 A - 2\nabla^2 A : \langle uuuu \rangle\right]$$

$$\underline{\underline{\kappa}} = (\nabla \underline{v})^T$$

2. A nonlocal stress tensor through "virtual work":

$$\delta W = \int_V \underline{\underline{\sigma}}^{(E)} : \delta \underline{\underline{\varepsilon}} \, dV = \delta F$$

Total Free Energy in V.



$\delta \underline{\underline{\varepsilon}}$ has to satisfy incompressibility.

The distottional part of free energy:

$$F_d = \nu \int_V dV \int d\underline{u} \left(\frac{1}{2} \psi U_{MG} \right)$$

$$\delta F_d = c \int_V (\nabla^2 A : \delta A + \delta \nabla^2 A : A) \, dV$$

$$\delta \nabla^2 A = \nabla^2 \delta A - \delta \varepsilon : \nabla \nabla A - \nabla \cdot (\delta \varepsilon \cdot \nabla A)$$

Eventually:

$$\underline{\underline{\sigma}}^{(E)} = 3 \nu \kappa T \Big[A - U (A \cdot A - A : \langle uuuu \rangle)$$

$$- \frac{U \mathcal{L}^2}{24} A \cdot \nabla^2 A - \langle uuuu \rangle : \nabla^2 A + \frac{Q - \nabla \nabla A}{4} \Big]$$

$$Q_{ij} = \frac{\partial A_{kl}}{\partial x_i} \frac{\partial A_{lk}}{\partial x_j} .$$

* Non-local
* Asymmetric
* Needs closure for $\langle uuuu \rangle$.