Heterogeneous Flows and Constitutive Behavior

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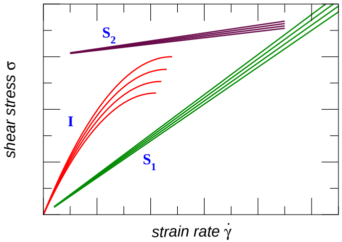
KITP, 18 January 2018

Phenomenology of shear banding [PDO EPL 1999]

Homogeneous constitutive relations for a hypothetical fluid:



I Newtonian:

S_1 flow-induced phase

S_2 flow-induced "gel"

- Identify dynamical variables (flow, composition, and structural information).
- "Phases" =steady state homogeneous solutions to equations of motion:

$$
\begin{aligned}
D_t\phi &= -\nabla\cdot M\nabla\mu(\phi, \boldsymbol{\nabla}\mathbf{v}, \mathbf{Q}) && = 0 && \text{(composition)}\\
\rho D_t\mathbf{v} &= \nabla\cdot\boldsymbol{\sigma}(\phi, \boldsymbol{\nabla}\mathbf{v}, \mathbf{Q}) && = 0 && \text{(flow)}\\
D_t\mathbf{Q} &= \mathcal{L}(\phi, \boldsymbol{\nabla}\mathbf{v}, \mathbf{Q}) && = 0 && \text{(microstructure)}
\end{aligned}
$$

- Calculate steady state flow curves as a function of concentration.

Stress-concentration couplings

- Two-fluid models [Helfand/Fredrickson 1989, Milner 1992], flow-induced migration [Leighton & Acrivos 1987, Schmidt/Marques/Lequeux PRE 1995].

$$\rho D_t \mathbf{v} = \nabla . G(\phi)\,\mathbf{W} - \phi\,\nabla \frac{\delta F(\phi)}{\delta \phi} + 2\,\nabla . \eta(\phi)\,\mathbf{D} - \nabla p_0,$$

$$D_t \phi = -\nabla \cdot \zeta^{-1}(\phi)\left[\nabla \cdot G(\phi)\mathbf{W} - \phi \nabla \frac{\delta F}{\delta \phi} + 2\,\nabla \cdot \eta(\phi)\,\mathbf{D}\right]$$

$$(\partial_t + \mathbf{v}_{\mathrm{m}} \cdot \nabla)\mathbf{W} + \ldots = +2\mathbf{D}_{\mathrm{m}} - \frac{\mathbf{W}}{\tau(\phi)} + \frac{\ell^2}{\tau(\phi)}\nabla^2\mathbf{W}$$

- Concentration builds up in more viscous regions.
- Polymer deformation in stress gradient.
- Transverse diffusion due to gradient in shear rate and hence collision rate; ....
- Migration in response to stress gradients imposed by geometry (e.g. Poiseuille flow).

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Careful:
- Total stress tensor $\mathbf{T} \neq \mathbf{T}_{\mathrm{micro}} - p\,\mathbf{I}$!!
- The pressure is given by $p = p_0 - \mathrm{Tr}(\mathbf{T}_{\mathrm{micro}})$.

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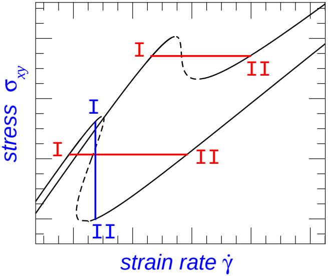
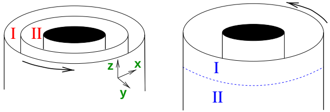
Geometry determines "field variables"

Definition of field and density variables depends on coexistence geometry.



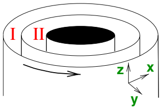


Phase separate according to $\bar{\phi} = \alpha\,\phi_I + (1-\alpha)\,\phi_S$.

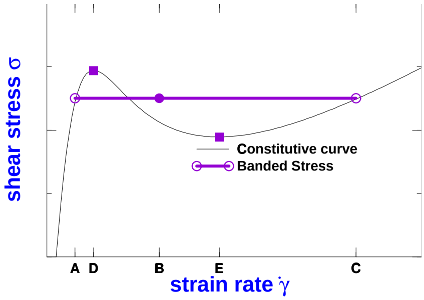
Common Stress	**Common Strain Rate**
Gradient Banding	Vorticity Banding
$\bar{\dot{\gamma}} = \alpha\,\dot{\gamma}_I + (1-\alpha)\,\dot{\gamma}_{II}$	$\bar{\sigma} = \alpha\,\sigma_I + (1-\alpha)\,\sigma_{II}$
$\sigma =$ "field variable"	$\dot{\gamma} =$ "field variable"
$\dot{\gamma} =$ "density variable"	$\sigma =$ "density variable"

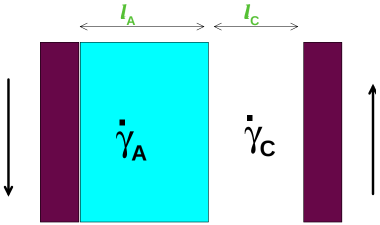
Coexistence Conditions: gradient banding [PDO Rheo Acta 2008]

1. Stationary states
2. Stress Balance



3. No ϕ flux:





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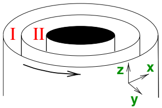

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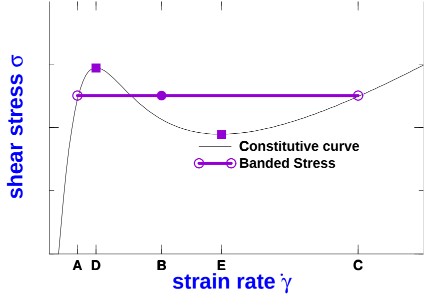

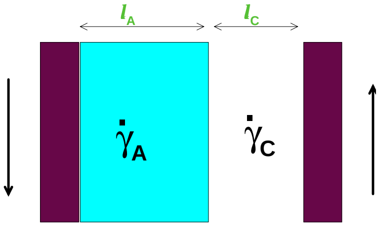

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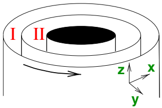
(uniform σ_{xy}, σ_{yy}) $\sigma^{\mathrm{I}}_{yy} = \sigma^{\mathrm{II}}_{yy} \Rightarrow p(y)$



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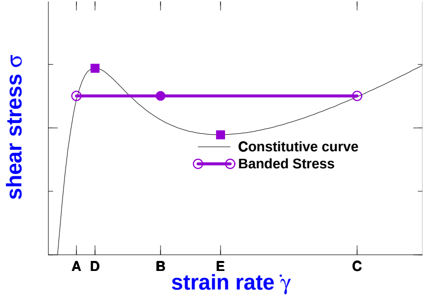

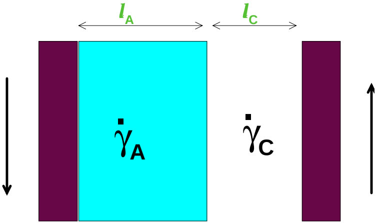

The pressure in the two bands may differ because of normal stress continuity.

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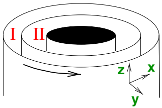
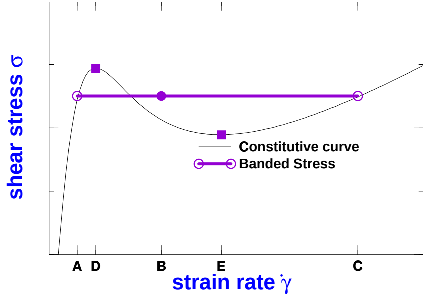
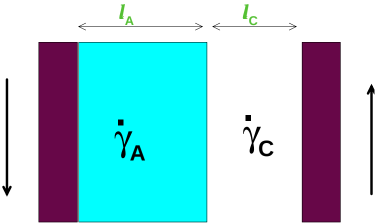
3. No ϕ flux: $\nabla \cdot \mathbf{J} = 0 \Rightarrow \quad \mu = \dfrac{\delta F}{\delta \phi} = \text{uniform}$







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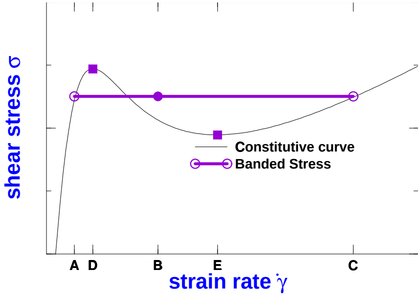
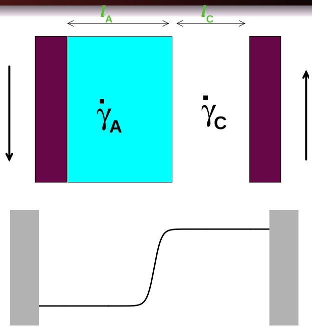
Stress selection and 'non-equilibrium phase coexistence'





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$$\partial_t \sigma_p = f(\sigma_p, \dot\gamma)$$

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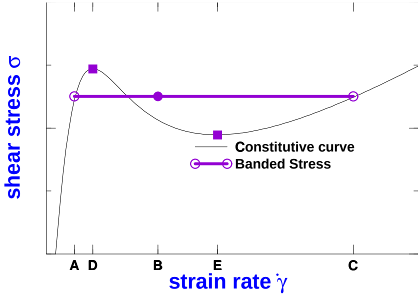

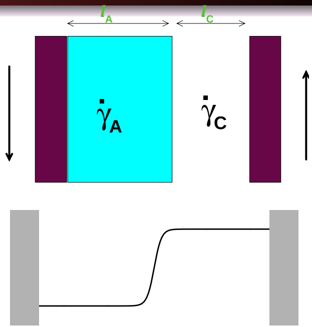

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- **Unique** $\mathcal{D}$-independent stress determined by inhomogeneous terms.

[PDO/PMG PRA 1992; Lu/PDO/Ball PRL 2000] – Concentration, finite stiffness, liquid crystallinity

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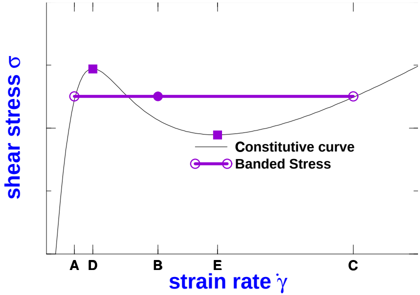

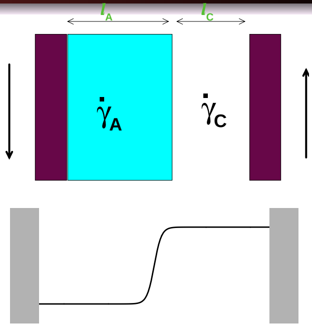

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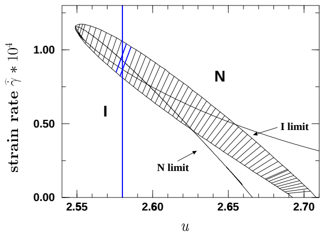
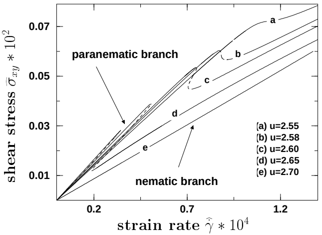
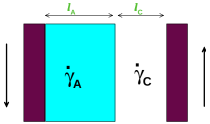
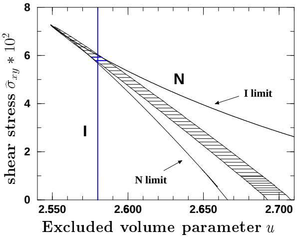
  [PDO/PMG PRA 1992; Lu/PDO/Ball PRL 2000] – Concentration, finite stiffness, liquid crystallinity
- The pressure difference can lead to an N_2-driven instability at a free meniscus and sample ejection [Skorski & PDO, 2011].

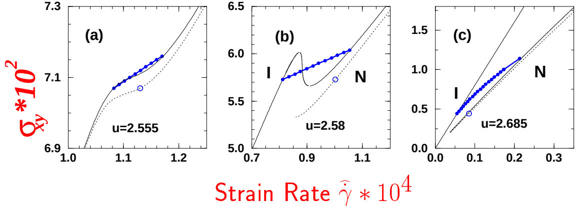
Liquid Crystals: Phase Diagram for Doi Model





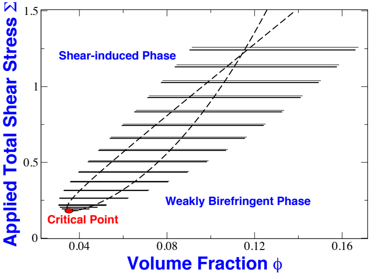


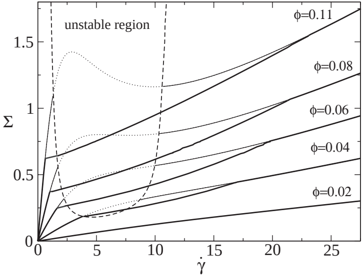




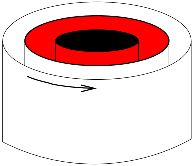
Wormlike Micelles [PDO, Radulescu, Lu JOR 2000, JNNFM 2000, PRL 2000]

Coupling to concentration fluctuations [Fielding/PDO, PRE 2003; EPJE (2003)]

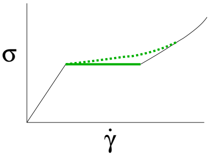




Common stress



(shear thinning)



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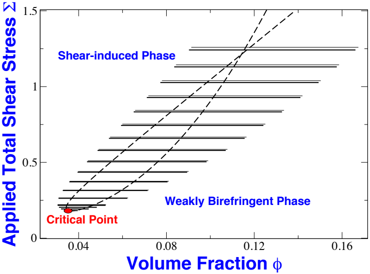
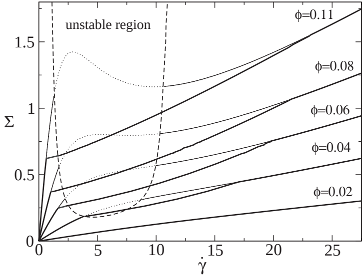
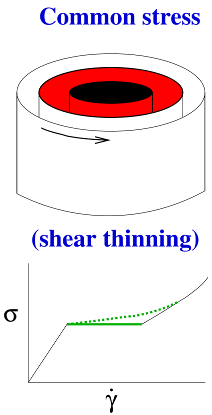
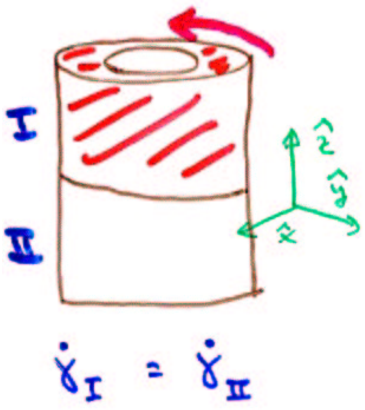






Note instability even with positive slope $d\Sigma/d\dot{\gamma} > 0$.

Coexistence Conditions: vorticity banding [PDO Rheo Acta 2008]



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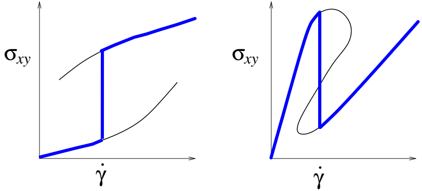

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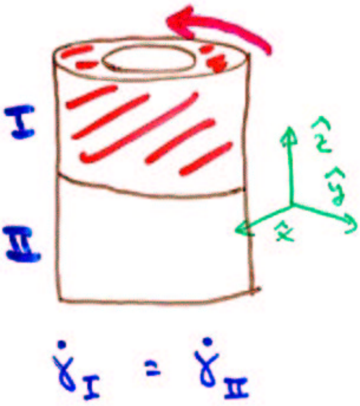

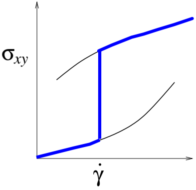

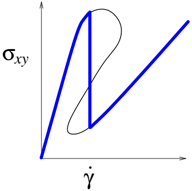

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\end{aligned}
$$

$$\nabla \cdot \boldsymbol{\sigma} = 0 \qquad\qquad \nabla \parallel \hat{\mathbf{z}}$$

$$\sigma^{\mathrm{I}}_{xz} = \sigma^{\mathrm{II}}_{xz}$$

$$\sigma^{\mathrm{I}}_{yz} = \sigma^{\mathrm{II}}_{yz}$$

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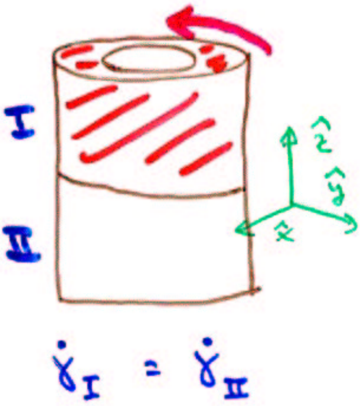

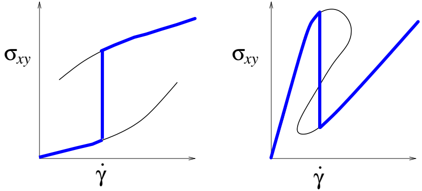

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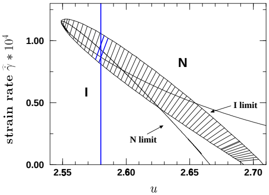
$$D_t\mathbf{Q} = 0 \qquad \dot\gamma \text{ branches}$$

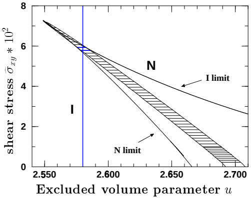
Inhomogeneous pressure $p(z)$;
measure $\sigma_{yy}(z)$; stable meniscus?

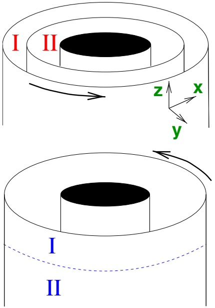
Calculations from a liquid-crystal model [PDO & Lu PRE 1997, 1999]

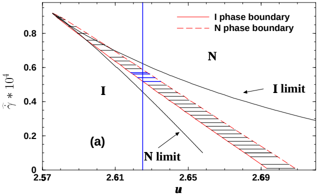
Gradient Banding

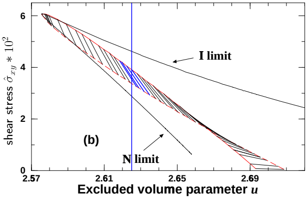
Vorticity Banding

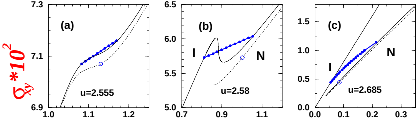


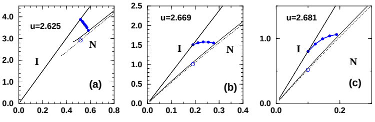




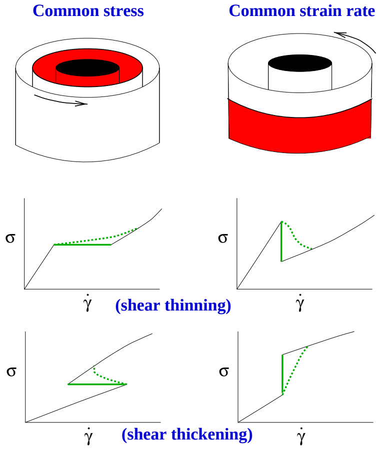








Typical Rheological Signatures of Banding [PDO, *Europhys. Lett.* (1999)]

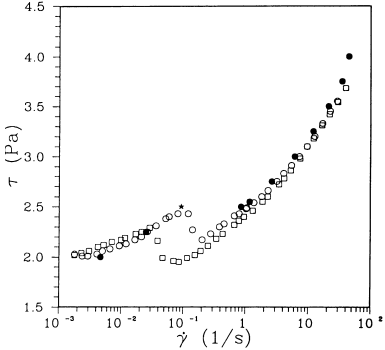


	Gradient	Vorticity
Thin	worms, liq. crystals	colloids, onions, sph. micelles
Thick	worms	onions DST?

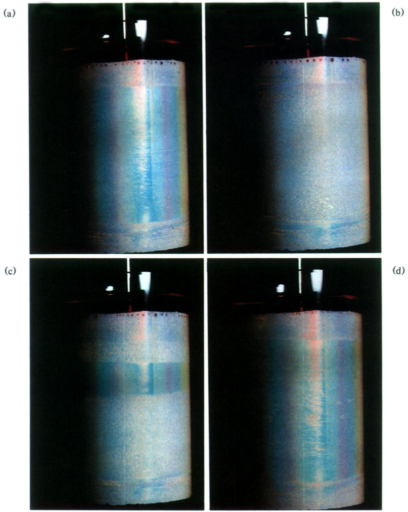
- Flat/Vertical plateaus: same concentration.
- Sloped plateaus: different coexisting concentrations [Schmitt *et al.* 1996].
- Vorticity banding: few examples, not well studied.

Colloidal Crystalline Suspensions [Chen, Zukowski *et al.* PRL 1992, Langmuir 1994].

$\phi = 0.45, 0.53;\ D = 230$ nm.



Polycrystalline +
ordered layer sliding.



Thinning Vorticity Banding

Colloidal Crystalline Suspensions [Chen, Zukowski *et al.* PRL 1992, Langmuir 1994].

$$\phi = 0.45, 0.53;\ D = 230 \text{ nm}.$$

2820 *Langmuir, Vol. 10, No. 8, 1994* *Chen et al.*

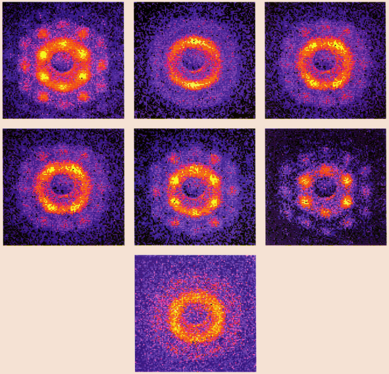
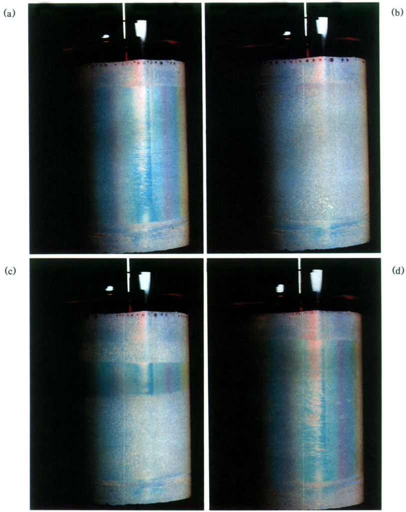
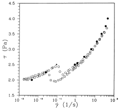


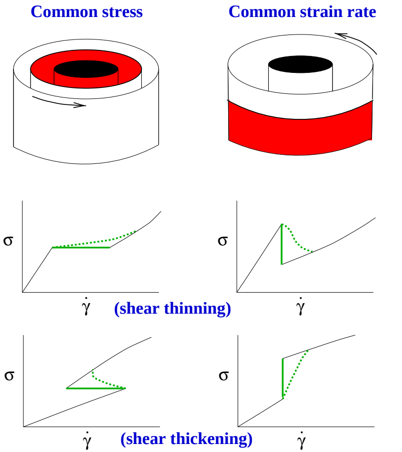
Figure 3. SANS scattering patterns with $\theta_c = 0$ at various shear rates: (a, top left) at rest, (b, top middle) 0.08 s^{-1}, (c, top right) 0.3 s^{-1}, (d, middle left) 15 s^{-1}, (e, middle middle) 40 s^{-1}, (f, middle right) 500 s^{-1}, (g, bottom) 6000 s^{-1}.



Polycrystalline +
ordered layer sliding.

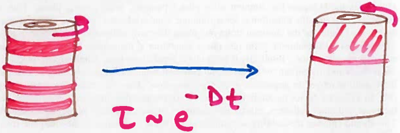


Kinetics during Vorticity Banding?



- No symmetry-breaking field.
- 1D coarsening ?

- Expect slow kinetics (in Couette)

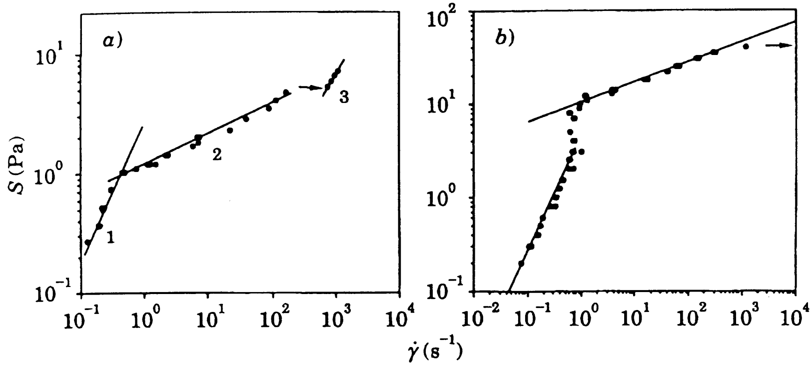


D: $\partial_t Q = \ldots\ldots + D\nabla^2 Q$

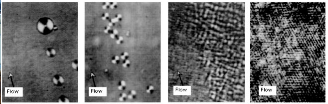
1D coarsening

- Curvature of Couette Flow accelerates coarsening of gradient banding

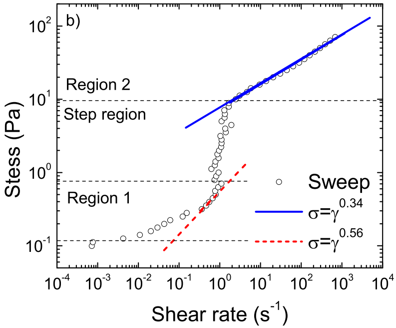
-

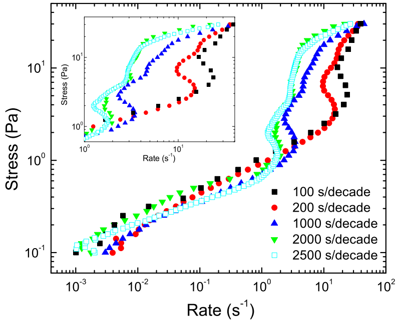


- SDS/dodecane/pentanol/water
  [Diat & Roux 1993]
- Candidate for vorticity banding on the (“stress cliff”)??



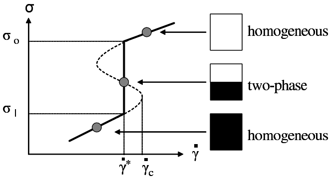
Onions in more detail [Wilkins & PDO EPJE 2006]





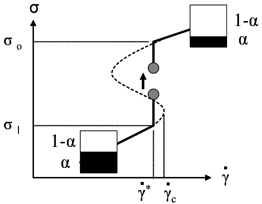
- No "Newtonian regime"
- Yield stress [smectic defect network?] and HB-like.
- Several transitions: vorticity bands?
- Hysteresis, slow transition.

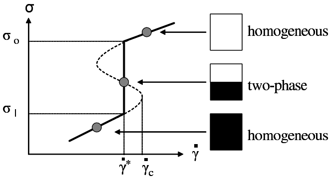
Cliff Region: Response to a stress jump $\sigma \to \sigma + \delta\sigma$?



$$\bar{\sigma}(\dot{\gamma}^*) = \alpha\,\sigma_O(\dot{\gamma})e + (1-\alpha)\,\sigma_L(\dot{\gamma})$$

Cliff Region: Response to a stress jump $\sigma \to \sigma + \delta\sigma$?

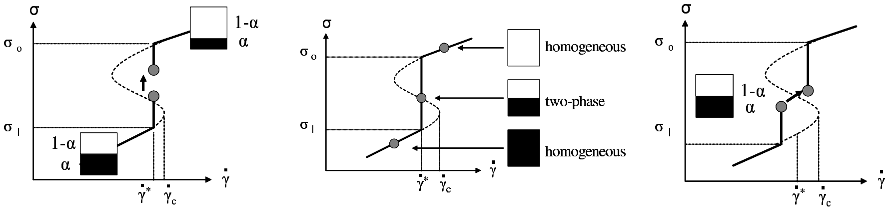




$$\bar{\sigma}(\dot{\gamma}^*) = \alpha\,\sigma_O(\dot{\gamma})e + (1-\alpha)\,\sigma_L(\dot{\gamma})$$

1. Nucleate more onions, $\alpha \to \alpha + \delta\alpha$ and return to selected strain rate.

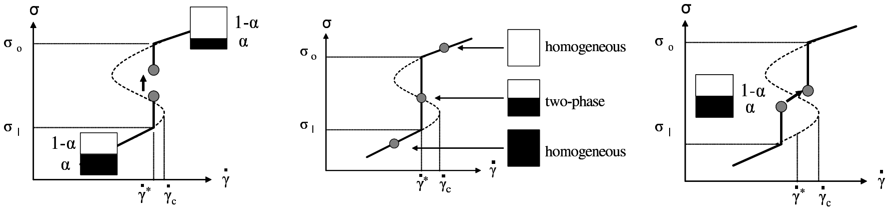
Cliff Region: Response to a stress jump $\sigma \to \sigma + \delta\sigma$?



$$\bar{\sigma}(\dot{\gamma}^*) = \alpha\, \sigma_O(\dot{\gamma})e + (1-\alpha)\, \sigma_L(\dot{\gamma})$$

1. Nucleate more onions, $\alpha \to \alpha + \delta\alpha$ and return to selected strain rate.
2. Resist nucleation, evolve strain rate $\dot{\gamma}^* \to \dot{\gamma}^* + \delta\dot{\gamma}$.

Cliff Region: Response to a stress jump $\sigma \to \sigma + \delta\sigma$?

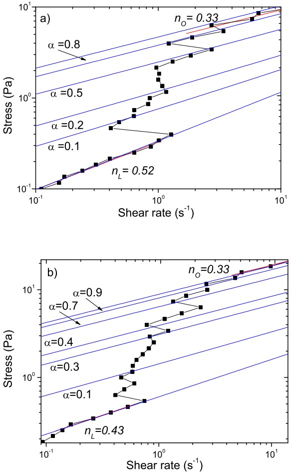


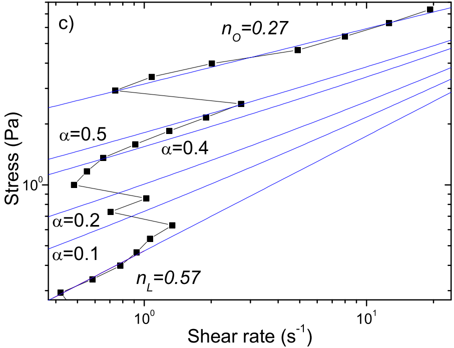
$$\bar{\sigma}(\dot{\gamma}^*) = \alpha\,\sigma_O(\dot{\gamma})e + (1-\alpha)\,\sigma_L(\dot{\gamma})$$

1. Nucleate more onions, $\alpha \to \alpha + \delta\alpha$ and return to selected strain rate.
2. Resist nucleation, evolve strain rate $\dot{\gamma}^* \to \dot{\gamma}^* + \delta\dot{\gamma}$.

- Nucleation/growth harder if vorticity banded:
  - different interface configuration (not under shear)
  - No driving force in Couette flow?.
  - Lamellae and onions cannot smoothly evolve to one another?

Scaling the Stress Cliff? [Wilkins & PDO EPJE 2006]



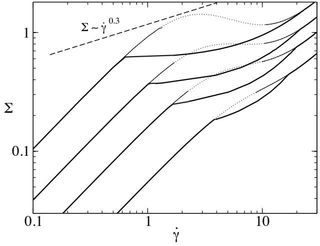


$$\bar{\sigma}(\dot{\gamma}^*) = \alpha\sigma_O(\dot{\gamma})e + (1-\alpha)\sigma_L(\dot{\gamma})$$

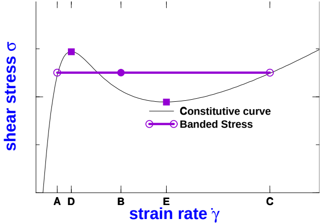
Instability of shearing flows [Fielding JOR 2016]

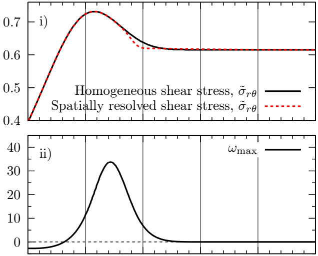
Overshoots imply instability......

- $\dfrac{d\sigma}{d\dot{\gamma}} < 0$ (constitutive)
- $\dfrac{d\sigma}{d\gamma} < 0$ (transient/dynamic)
- concentration/order coupling



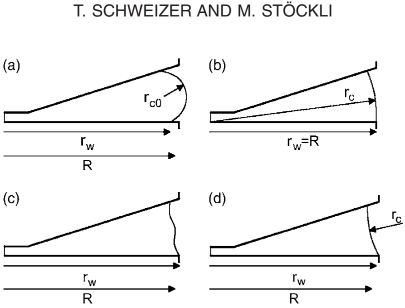
[Fielding & PDO, 2003]





[Adams & PDO, PRL 2008]

Boundary Effects



[Schweizer & Stöckli JOR 2008]

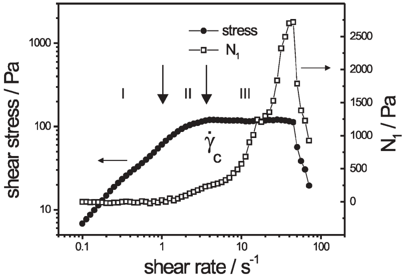
- Free surface balance
- Edge fracture
- Wall slip
- Instability in cone & plate and Couette flows.
- Stress gradient in channel/Poiseuille flows.

Can shear banding induce edge fracture? [Skorski and PDO, JOR (2011)]

Edge fracture for $|N_2| > \frac{\gamma}{R}$ [Tanner & Keentok, JOR 1983, Hemingway & Fielding arXiv:1703.05013].

Wormlike Micelles

[Lopez-Gonzalez, Soft Matter 2006]



Polymer Solutions

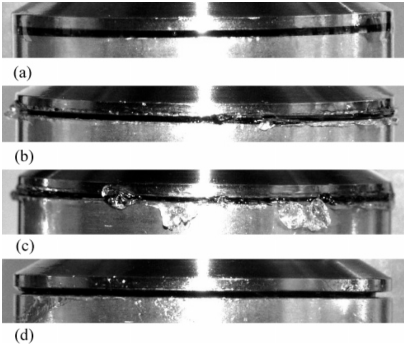
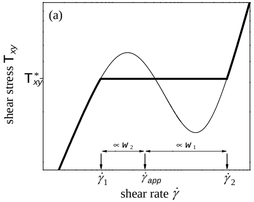


Figure 2. Pictures of the meniscus (a) after sample loading, (b) during the initial transient following step-up to 2500 Pa, (c) during the final portion of the transient, and (d) with extruded material removed from the exterior of the fixture. The pictures were taken without temperature control by the Peltier plate for better visualization of the meniscus shape.

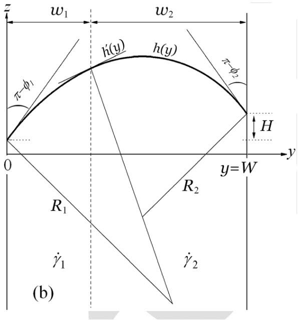
[Inn, Wissbrun, and Denn, Macromolecules 2005].

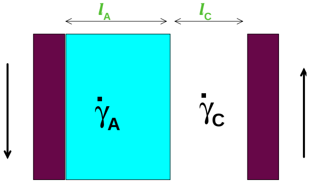
Surface tension γ vs. normal stress balance:

$N_2 = T_{yy} - T_{zz}$



side view





Top view

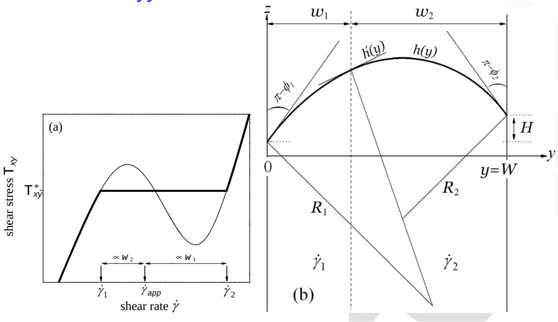
- Normal stress balance at meniscus:

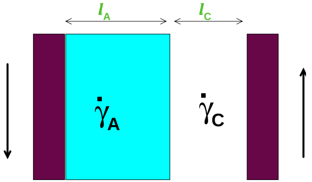
$$\Delta N_2 = \Delta\left(\frac{\gamma}{R}\right)$$

Surface tension γ vs. normal stress balance:

$$N_2 = T_{yy} - T_{zz}$$

side view





Top view

- Normal stress balance at meniscus:

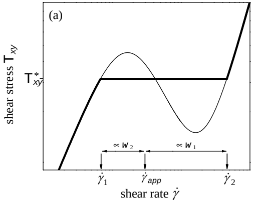
$$\Delta N_2 = \Delta\left(\frac{\gamma}{R}\right)$$

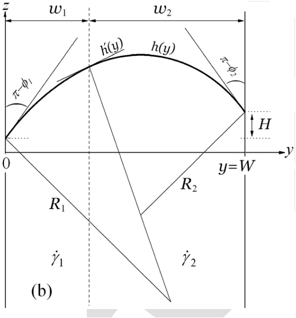
- Fixed contact angle ϕ.

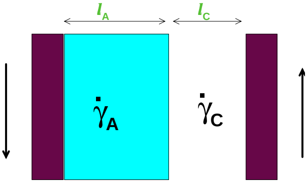
Surface tension γ vs. normal stress balance:

$$N_2 = T_{yy} - T_{zz}$$

side view







Top view

- Normal stress balance at meniscus:

$$\Delta N_2 = \Delta\left(\frac{\gamma}{R}\right)$$

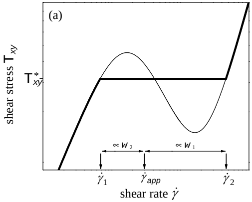
- Fixed contact angle ϕ.
- Control parameter:

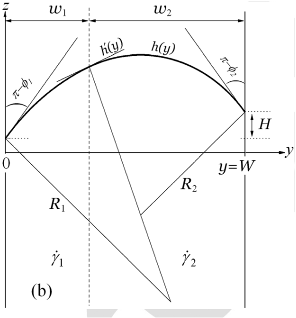
$$A = \frac{LG}{\gamma}\frac{\Delta N_2}{G}.$$

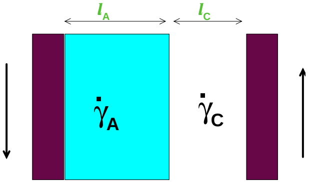
Surface tension γ vs. normal stress balance:

$N_2 = T_{yy} - T_{zz}$

side view







Top view

- Normal stress balance at meniscus:

$$\Delta N_2 = \Delta\left(\frac{\gamma}{R}\right)$$

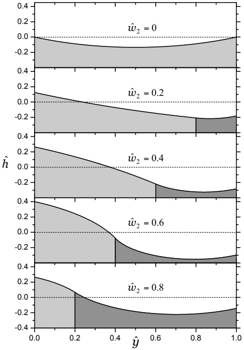
- Fixed contact angle ϕ.
- Control parameter:

$$A = \frac{LG}{\gamma}\frac{\Delta N_2}{G}.$$

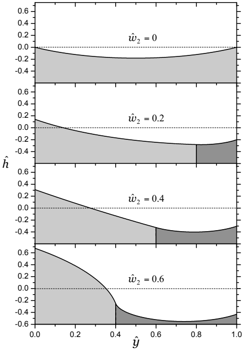
- Elastocapillary length

$$\xi_e = \gamma / G.$$

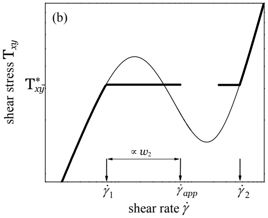
Meniscus profiles acrosss the plateau – Instability

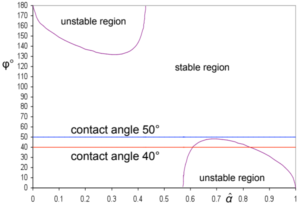


$\phi = 60°$



$\phi = 40°$

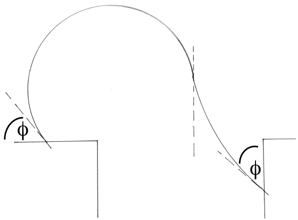


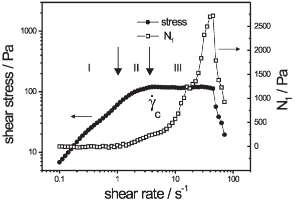


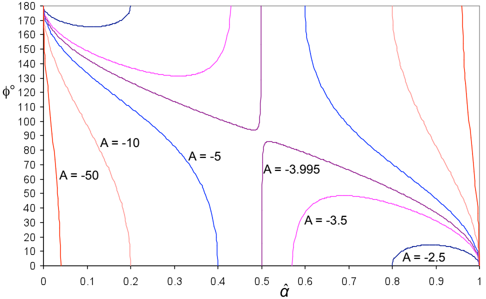
$$A = \frac{LG}{\gamma}\frac{\Delta N_2}{G} = -3.5$$

Instabilities: $A = LG\Delta N_2/\gamma G$

Expulsion





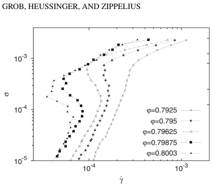


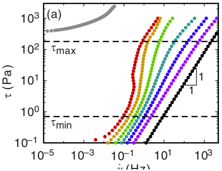
	A	< -4		Unstable
$-4 <$	A	< -2		Unstable or stable
$-2 <$	A	< 0		Stable

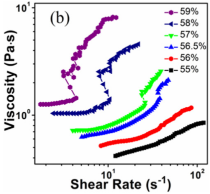
$$-A \simeq \begin{cases} 10 - 100 & \text{polymer solutions} \\ 0.5 - 4 & \text{wormlike micelles} \end{cases}$$

Vorticity Banding: DST in colloids?

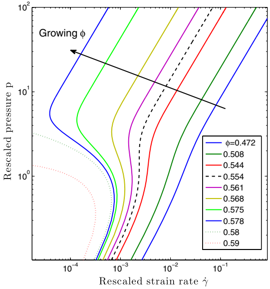
[Grob et al., PRE 2013, Brown & Jaeger Rep Prog Phys 2014, Pan et al. PRE 2015]

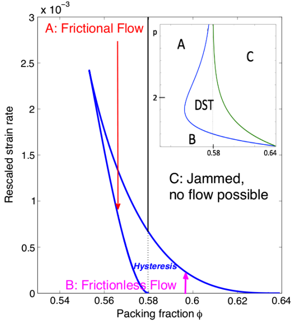




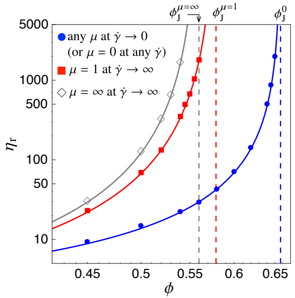


[Wyart & Cates PRL 2014]

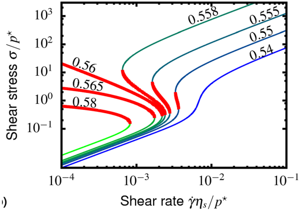




Wyart/Cates model (non-Brownian suspensions) [PRL 2014]



[Seto et al., PRL 2013, JOR 2014]



[Guy et al., JOR 2016]

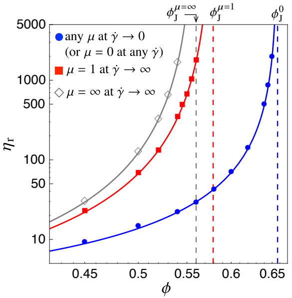
[Seto, Mari, Denn, Morriss, Cates, Wyart, ...]

Viscosity
$$\eta = \frac{1}{\left(1 - \frac{\phi}{\phi_J(p_p)}\right)^2}$$

Jamming
$$\phi_J = \phi_m f(p_p) + \phi_0(1 - f(p_p))$$

Contacts
$$f(p_p) = (1 - e^{-p_p/p^*})$$

Wyart/Cates model (non-Brownian suspensions) [PRL 2014]



[Seto, Mari, Denn, Morriss, Cates, Wyart, ...]

Viscosity
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$$\phi_J = \phi_m f(p_p) + \phi_0(1 - f(p_p))$$

Contacts
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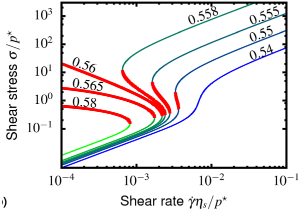
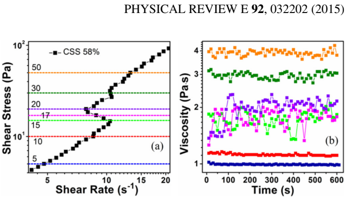


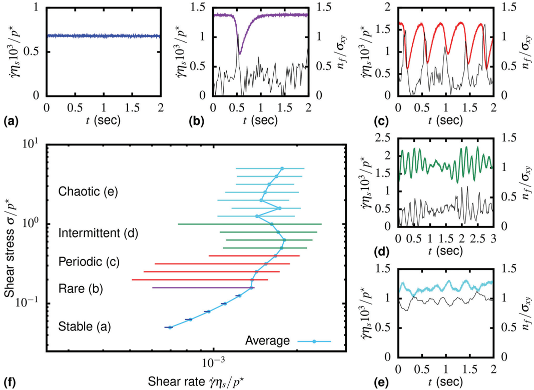
[Guy et al., JOR 2016]

- Correct choice of fabric tensor **A**?
- Orientational order?
- $\mathbf{T} = \mathbf{T}(\mathbf{A}, f, \mathbf{D}, \ldots)$
- Dynamics $\partial_t f = \ldots, \partial t\, \mathbf{A} = \ldots$?
- Frictional models are non-analytic and non-differentiable!

Unsteady vorticity banding in non-Brownian suspensions?



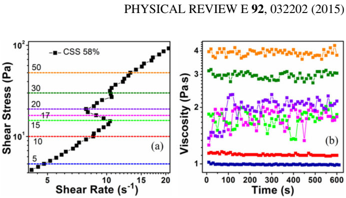
[Pan, de Cagny, Weber and Bonn, PRE 2015]

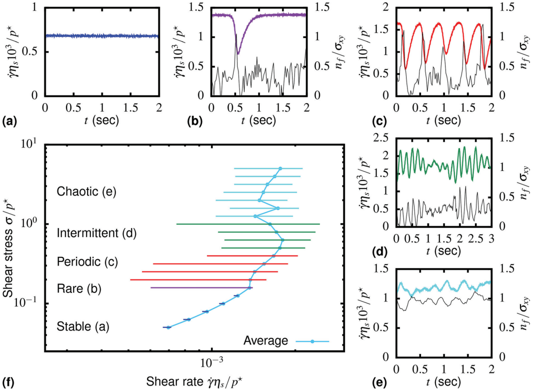


[Hermes et al., JOR 2016]

- Unsteady bands: cannot separately balance particle stress $p_{p,zz}(f,\phi)$ *and* solvent pressure at the interface? General feature for non-Brownian suspensions?

Unsteady vorticity banding in non-Brownian suspensions?





[Pan, de Cagny, Weber and Bonn, PRE 2015]

[Hermes et al., JOR 2016]

- Unsteady bands: cannot separately balance particle stress $p_{p,zz}(f, \phi)$ *and* solvent pressure at the interface? General feature for non-Brownian suspensions? What about the meniscus? [open boundaries in expts]

Final thoughts.....

There are many models for yielding materials (fluids and solids); usually these are not treated at a particle level.

- STZ-motivated models [Lemaitre, Langer, Manning, Falk, ...]
- Long-range elastic/viscoplastic models [Picard, Lequeux, Ajdari, Martens, Barrat, ...]
- Fluidity models [Bonn, Mansard/Colin, Ovarlez, Coussot, ...] .

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