Designing a Cross-Slot for Extensional-FlowSANS

Shooting Neutrons at Soap

Koty McAllister (UD, NCNR SURF), Katie Weigandt (NCNR)

Complex Fluids and Flow

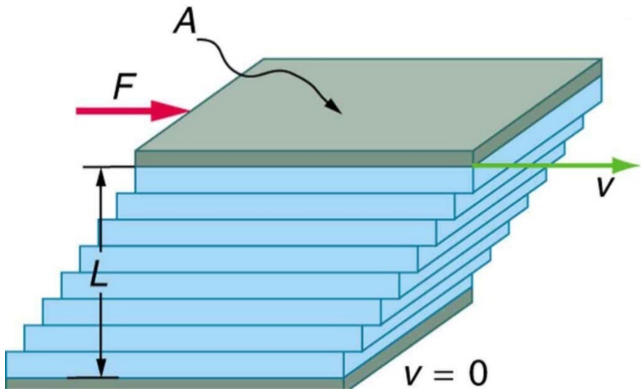
Consumer Products

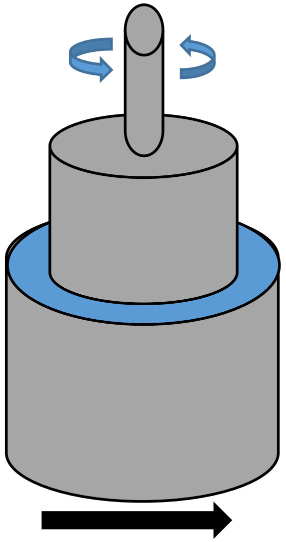
Polymer processing and extrusion

Processing and delivery of pharmaceuticals

Shear and Extensional Flow

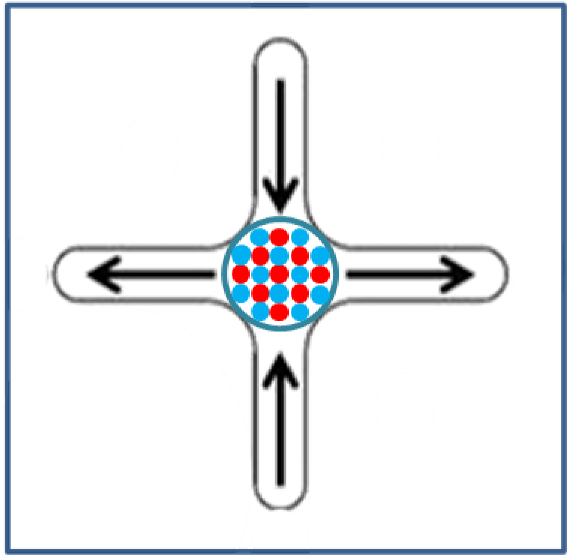
Shear Strain

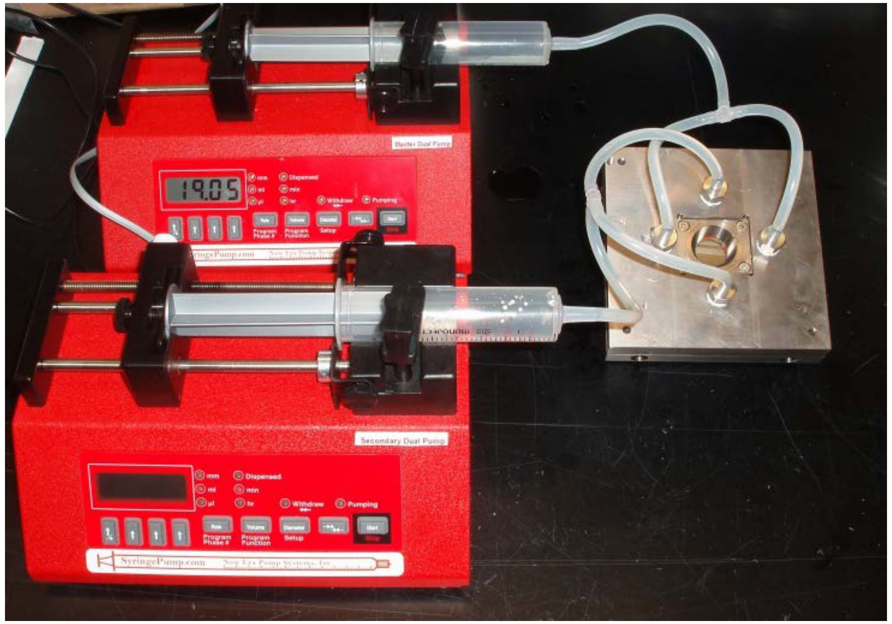


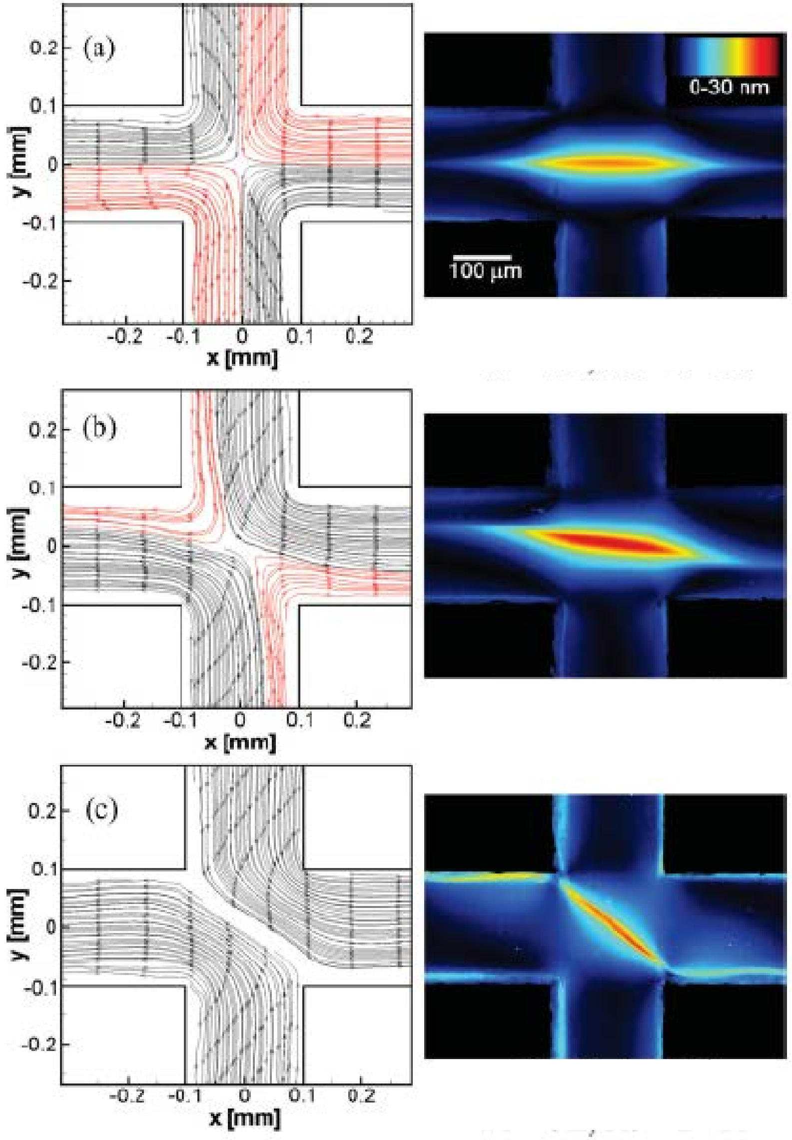


Extensional Strain

Cross-Slot Flow Cell

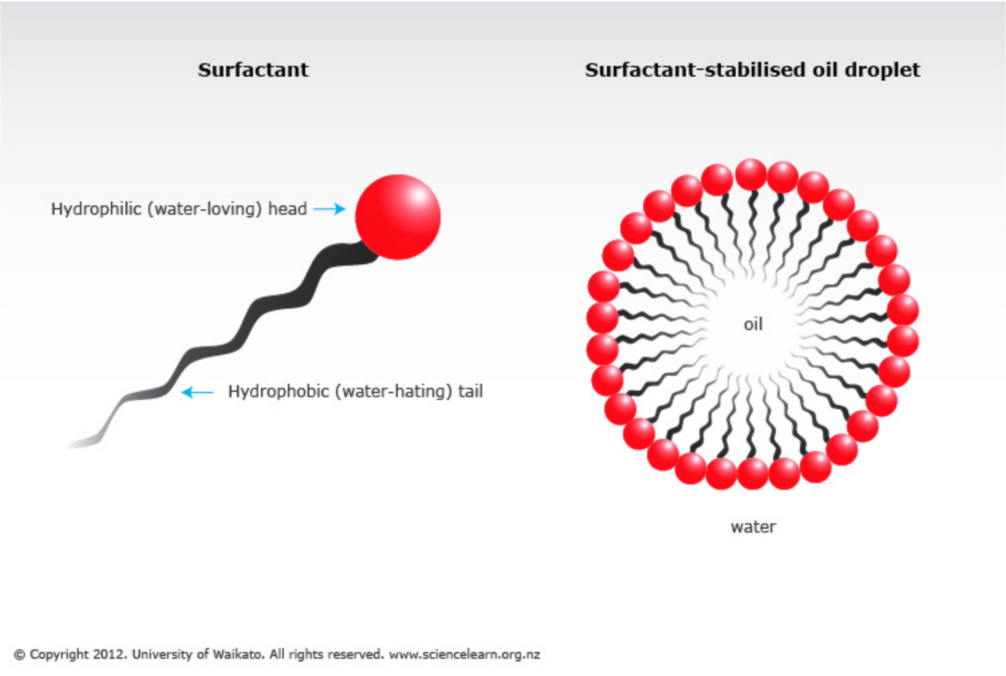




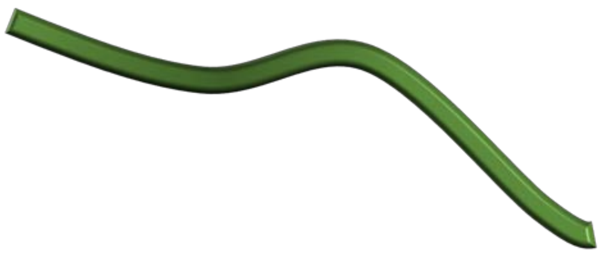


Haward, S.; McKinley, G. *Physical Review.* **2012**, 85, 031502-1-031502-14

Wormlike Micelles (WLM)



From University of Waikato, January 11, 2012, sciencelearn.org.nz



75mM CPyCl/ 45 mM NaSal in D_2O

$$\tau_r \approx 7\ sec$$

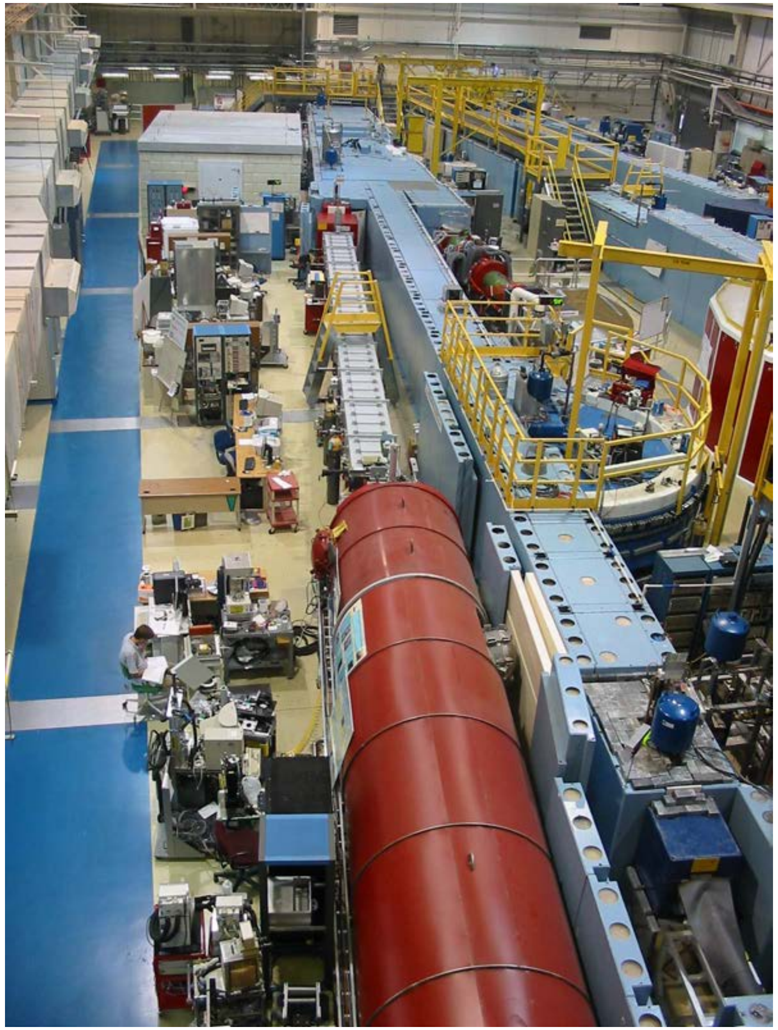
Personal care products

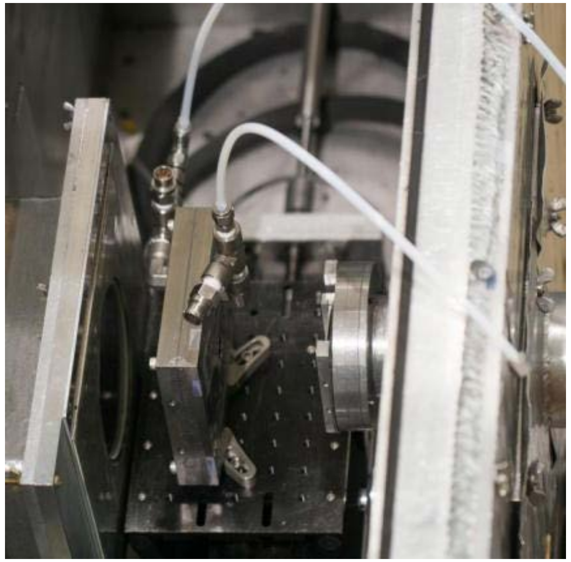
Home care products

Oil recovery and fracking

Drag reducers

Small Angle Neutron Scattering





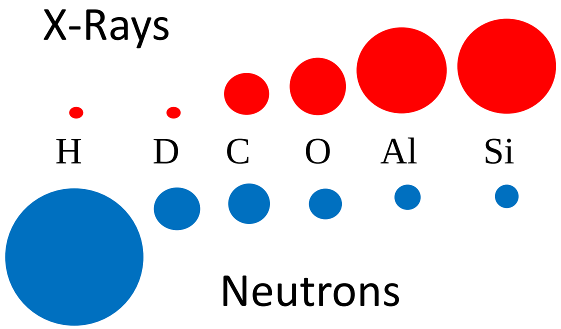
NCNR."NG7."www.ncnr.nist.gov

Why Small Angle Neutron Scattering?

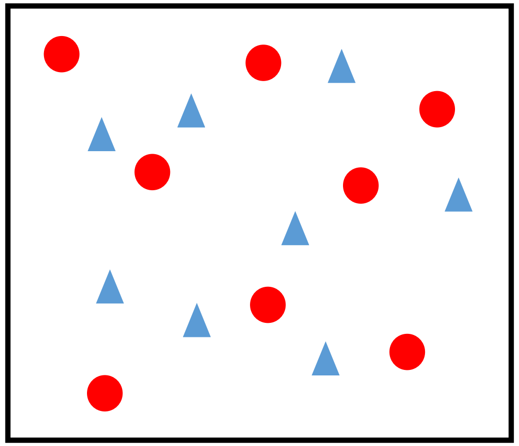
Characterize structures from 1 nm – 500 nm

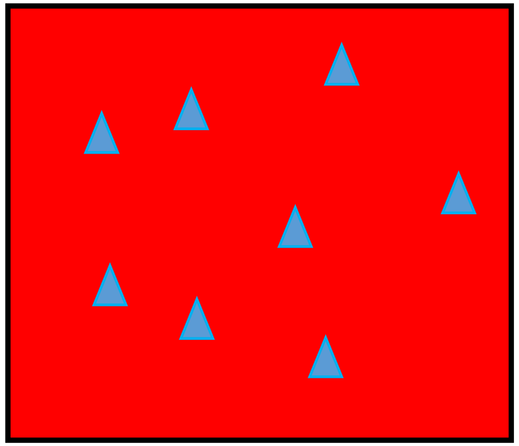
Transparency

Scattering Cross-Sections

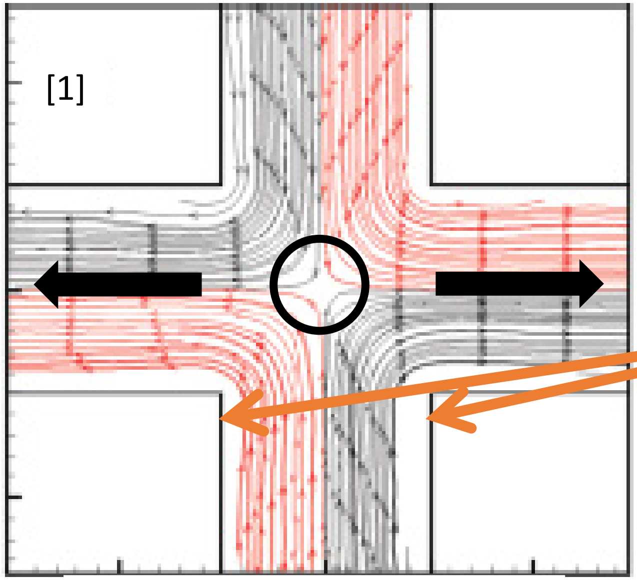


Contrast Variation





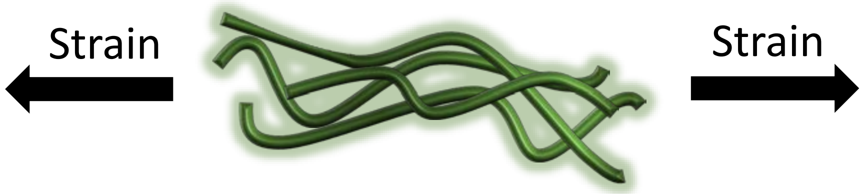
Extensional Flow within a Cross Slot



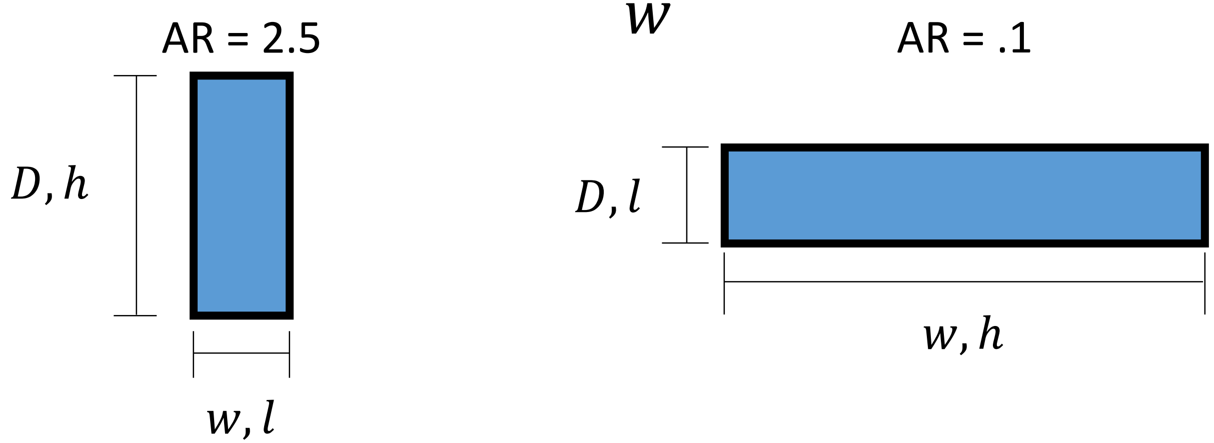
Plug-like flow:

$$\dot{\epsilon}_{nom} = \frac{Q}{w^2 D} \text{ [1]}$$

$$\dot{\gamma}_{wall} = \frac{6Q}{l^2 h}; l < h$$ (Newtonian Fluid)



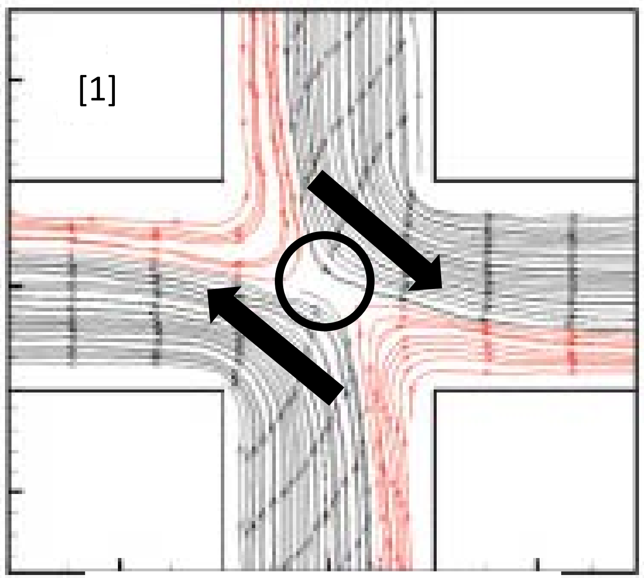
$$AR = \frac{D}{w}$$

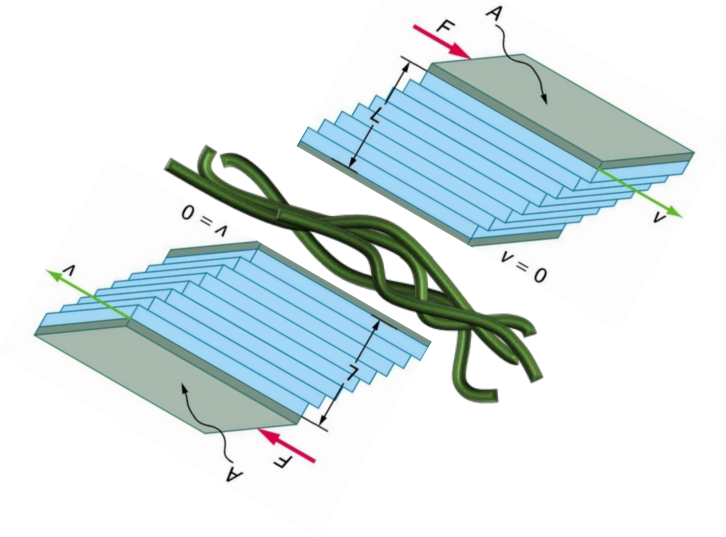


Aspect ratios of 2.5, 1.7, 1, 0.7, 0.1

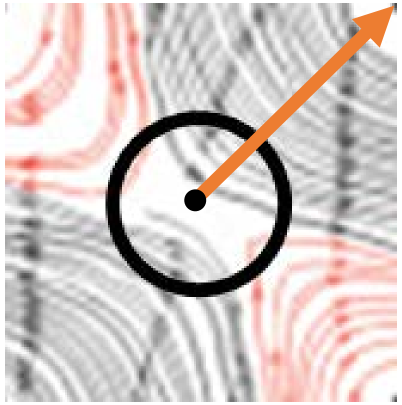
[1] Haward, S.; McKinley, G. *Physical Review.* **2012**, 85, 031502-1-031502-14
J. Penfold, I. Tucker. *J. Phys. Chem. B.* **2007**, 111, 9496-9503

Asymmetric Flow within a Cross Slot

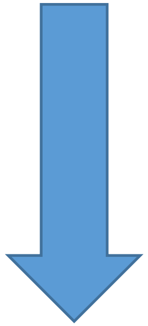


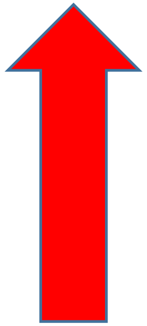


Occurs when $\dot{\epsilon} > \dot{\epsilon}_c$



$\dot{\epsilon}$

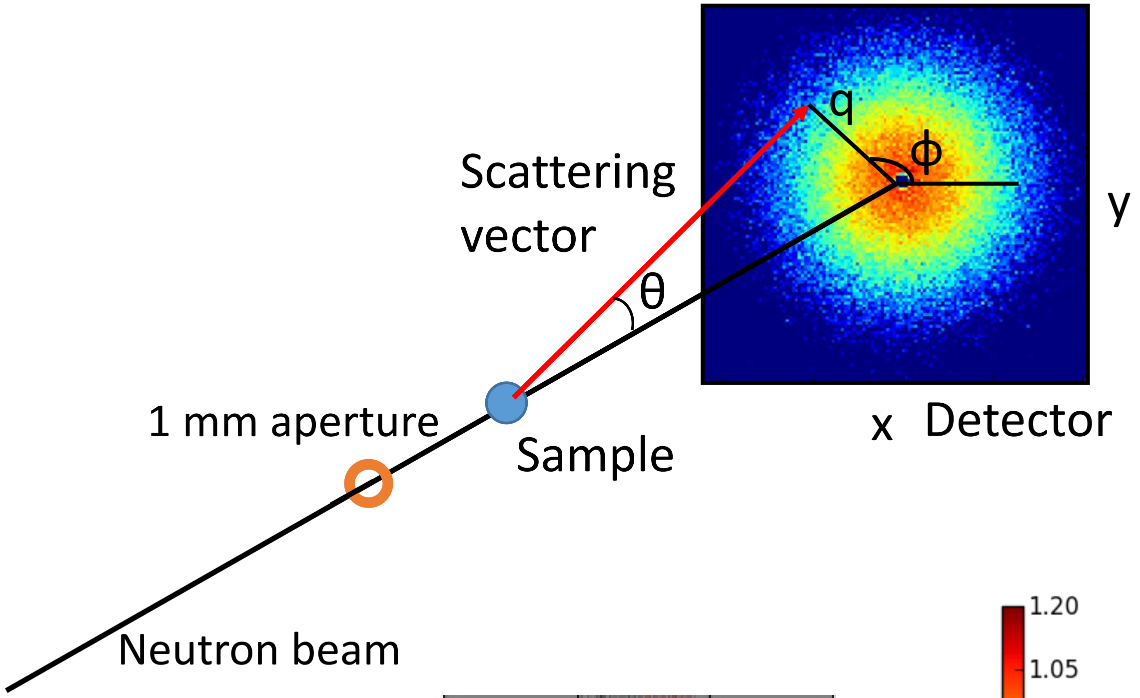




$\dot{\gamma}$

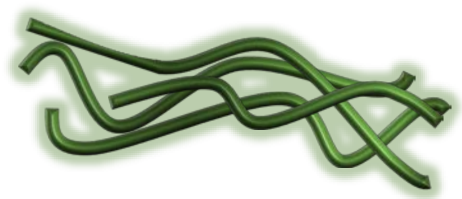
[1] Haward, S.; McKinley, G. *Physical Review.* **2012**, 85, 031502-1-031502-14

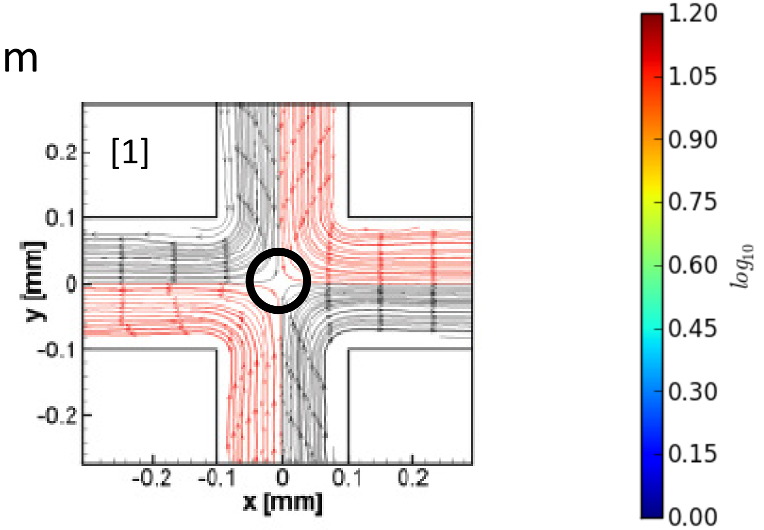
Small Angle Neutron Scattering (SANS)

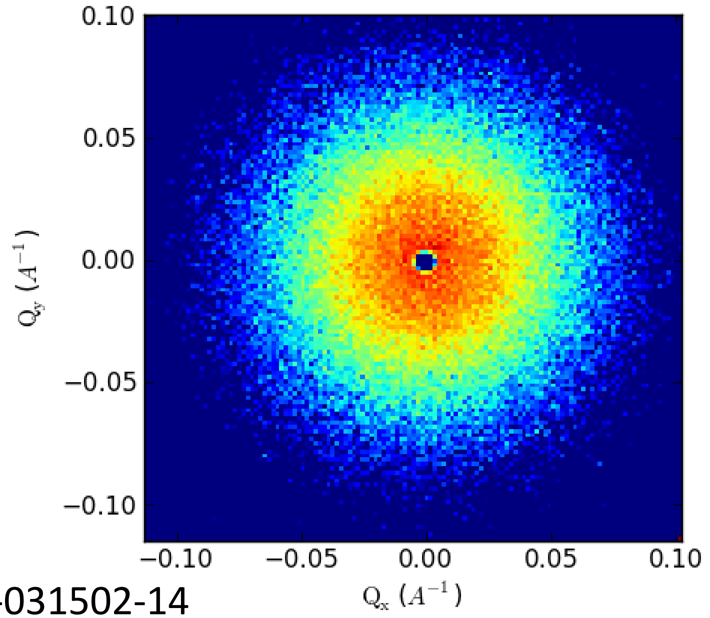


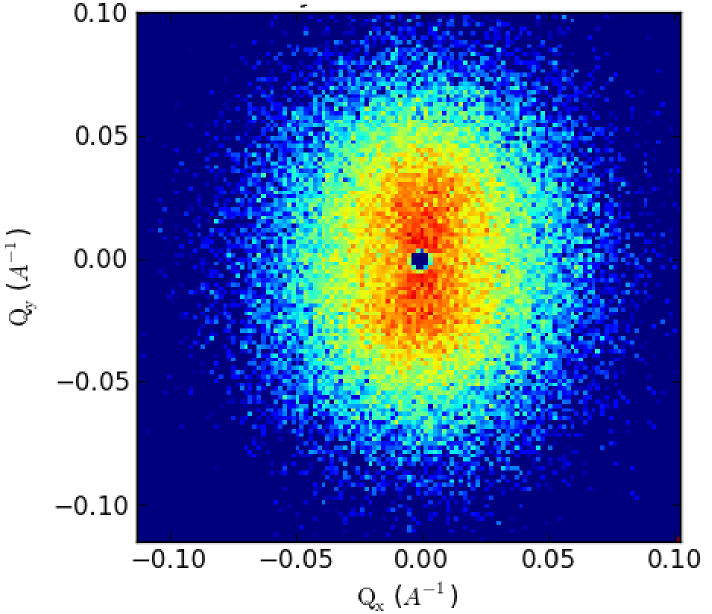
Isotropic

Anisotropic







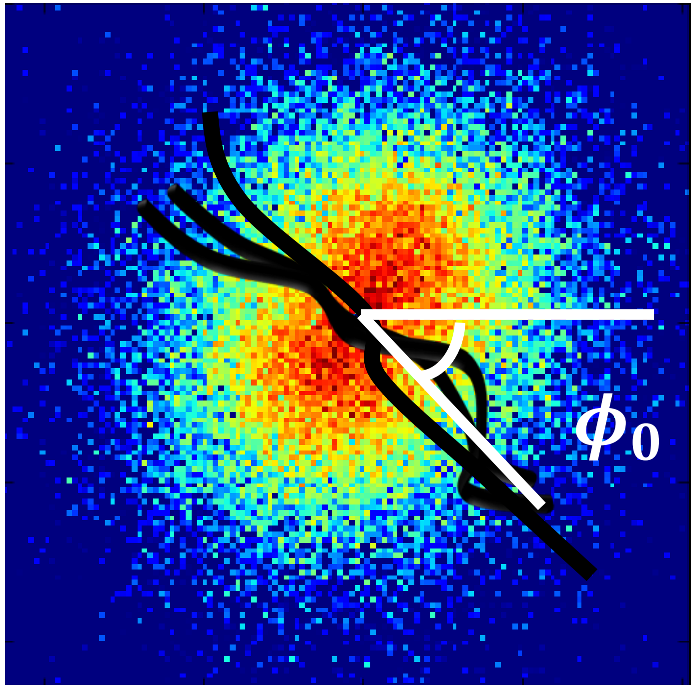


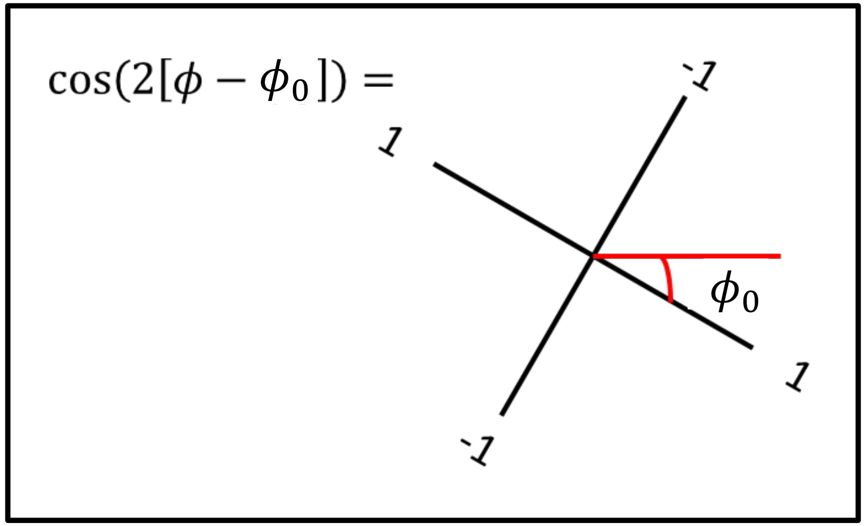
[1] Haward, S.; McKinley, G. *Physical Review.* **2012**, 85, 031502-1-031502-14

Alignment Factor

$$A_f(q) = \frac{\int_0^{2\pi} I(q,\phi)\cos(2[\phi-\phi_0])\,d\phi}{\int_0^{2\pi} I(q,\phi)\ d\phi}$$

$$-A_f(q \geq 0.03\ A^{-1}) \approx S_m{}^{[2]}$$





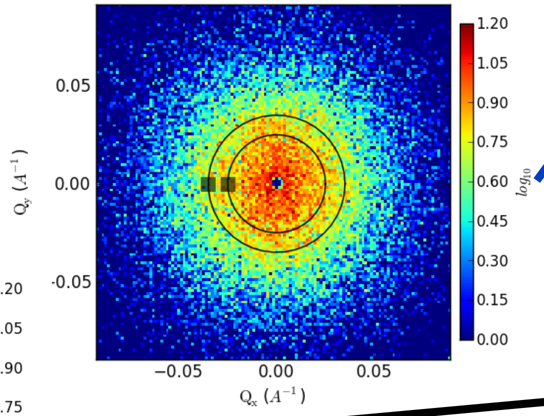
[2] L.M. Walker, "Rheology and Rheo-optics of liquid crystal polymers under flow." **1995**

Nematic Orientation Parameter

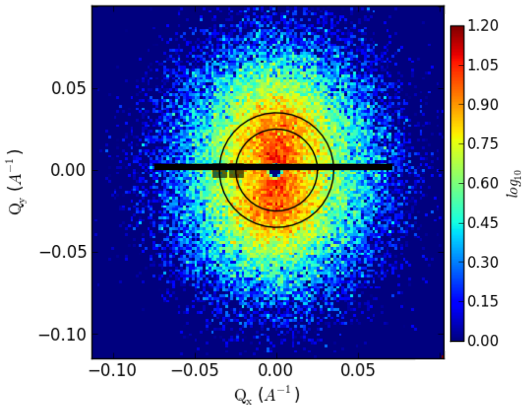
$$I(\phi) = \sum_{n=0}^{\infty}\left\{\frac{(-1)^n(2n)!}{4^n n!\,n!} a_n P_{2n}(\cos(\phi - \phi_0))\right\}$$

$$\bar{P}_2 = \frac{a_1}{5a_0}$$

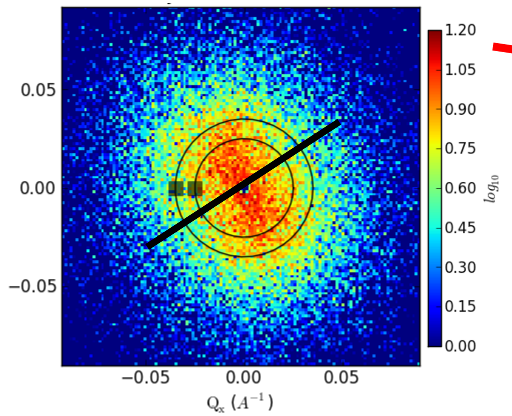
$\bar{P}_2 = 0.0321$
$\phi_0 = N/A$



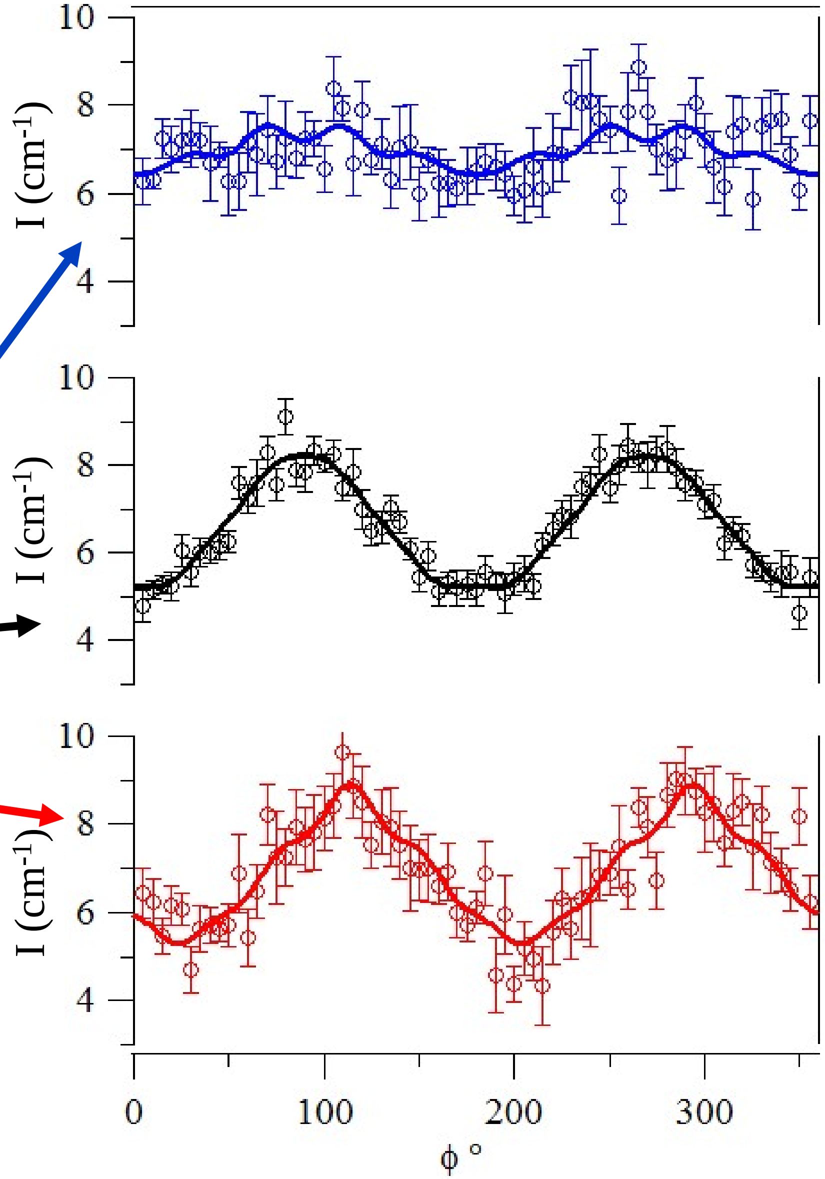
$\bar{P}_2 = 0.1224$
$\phi_0 = -0.4°$



$\bar{P}_2 = 0.1127$
$\phi_0 = 24°$



Annular averages take at $q = 0.03\ A^{-1}$



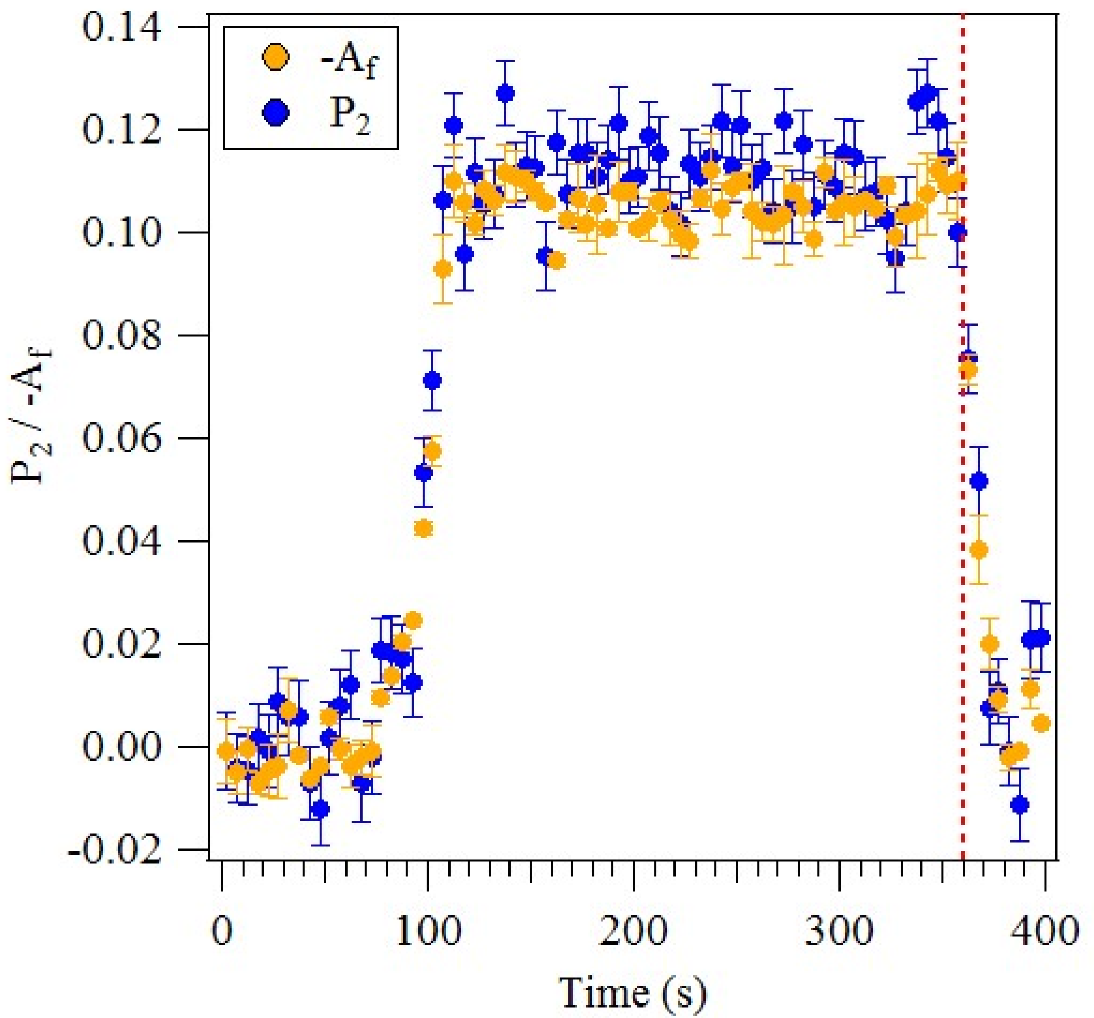
$\overline{P_2}$ and A_f

ODF: $g(\beta) = \sum_{n=0}^{\infty} a_n P_{2n}(cos\beta)$

$\bar{P}_2 = \left\langle \frac{3cos^2(\beta)-1}{2} \right\rangle = 1 - \frac{3}{2}\overline{sin^2(\beta)} = S_m$[3]

Therefore $\bar{P}_2 \approx -A_f \; (q \geq 0.03 \; A^{-1})$

Data from $\dot{\epsilon} = 0.8 \text{ s}^{-1}$, AR = 2.5, 5 sec bins

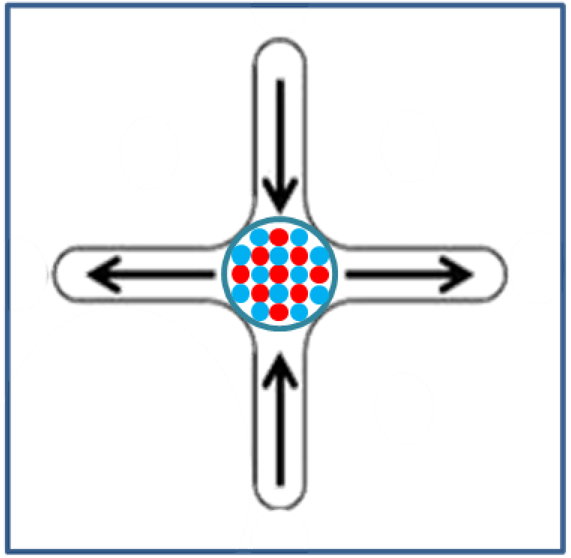


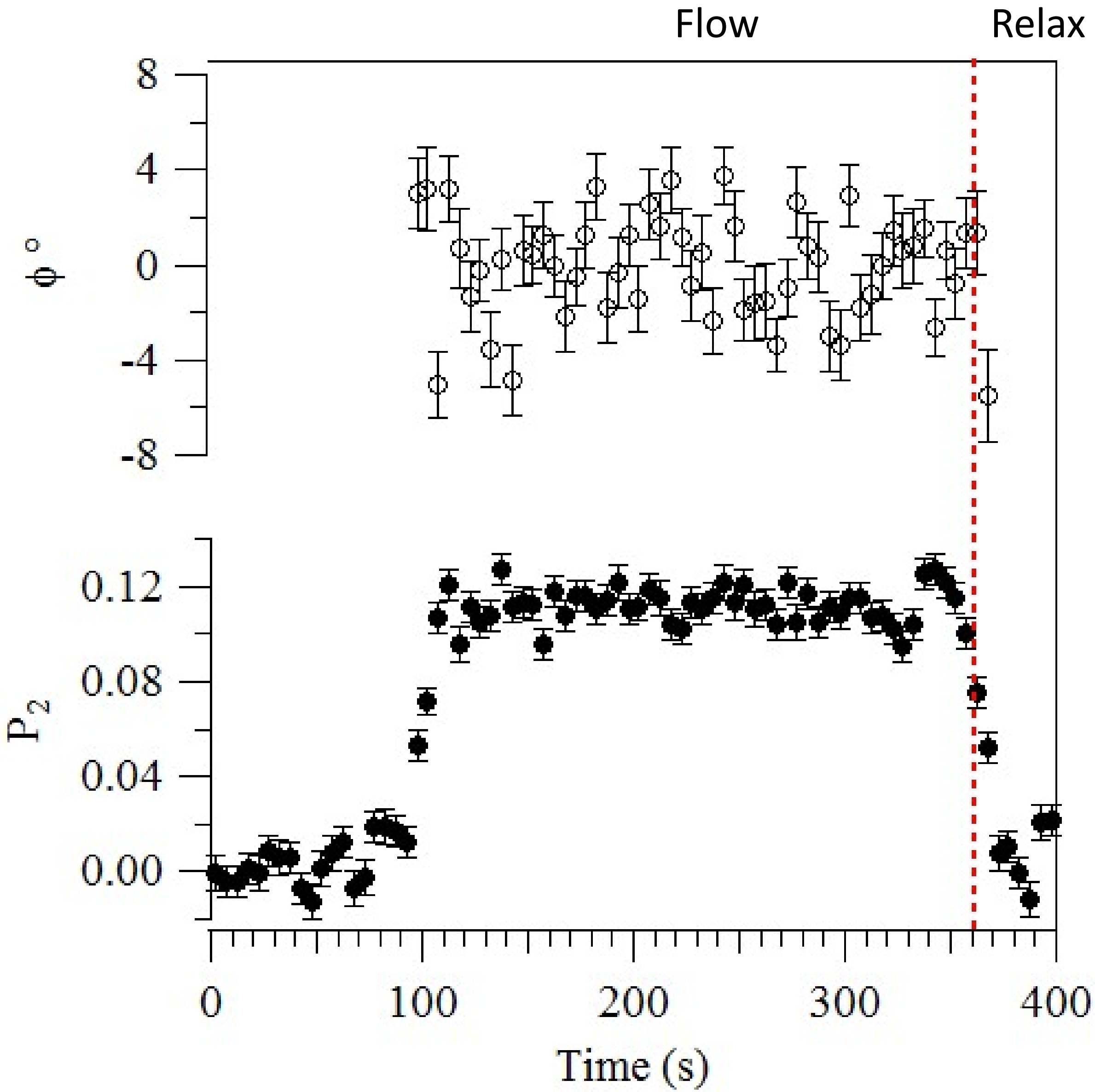
[3] W. H. DeJeu, *Mol. Cryst. Liq. Cryst*. **1997,** 292, 13.

$\dot{\epsilon} = 0.8\ s^{-1}$ Time Resolved

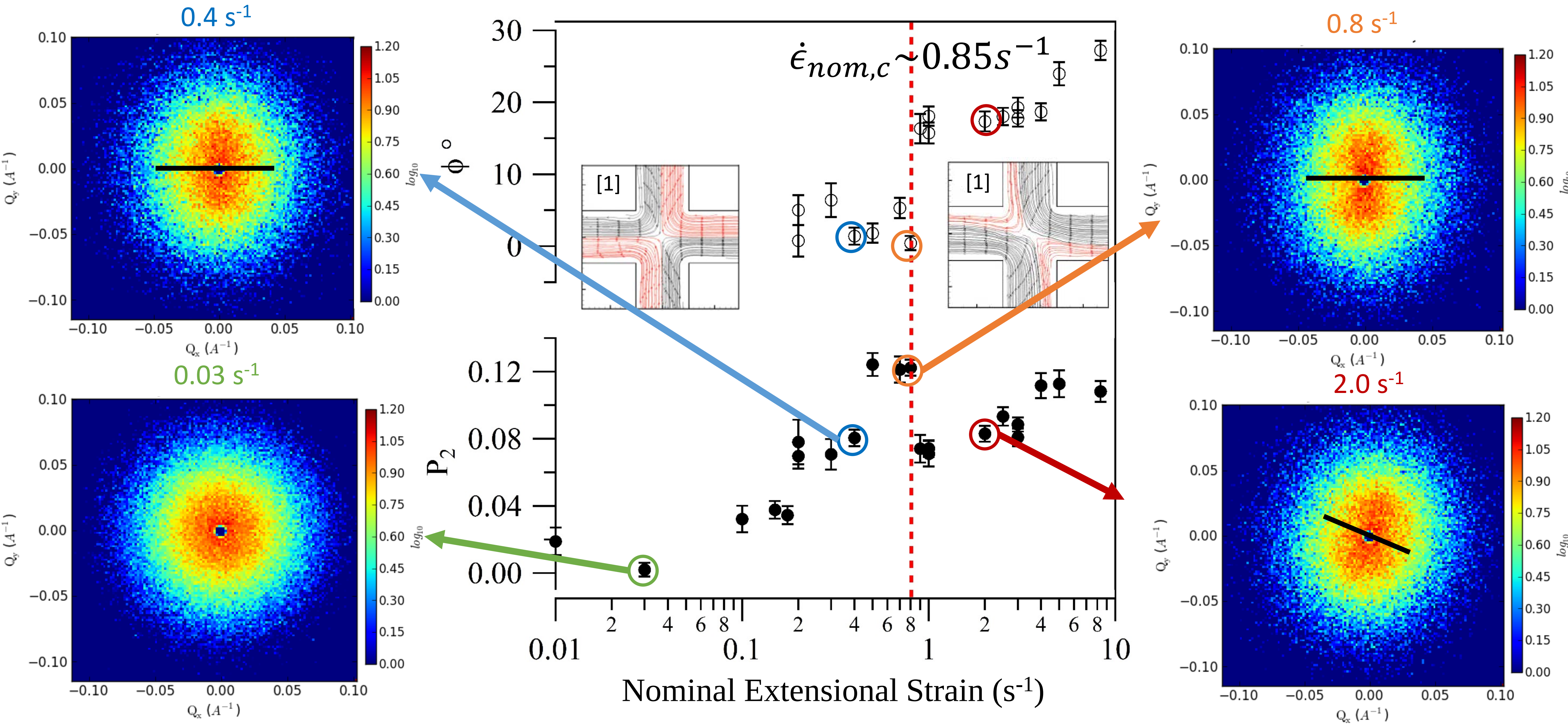
Steady state orientation is reached after ~110s

$$\bar{P}_2 = 0.12$$
$$\phi_0 = 0$$





Equilibrium Structure (AR=2.5)

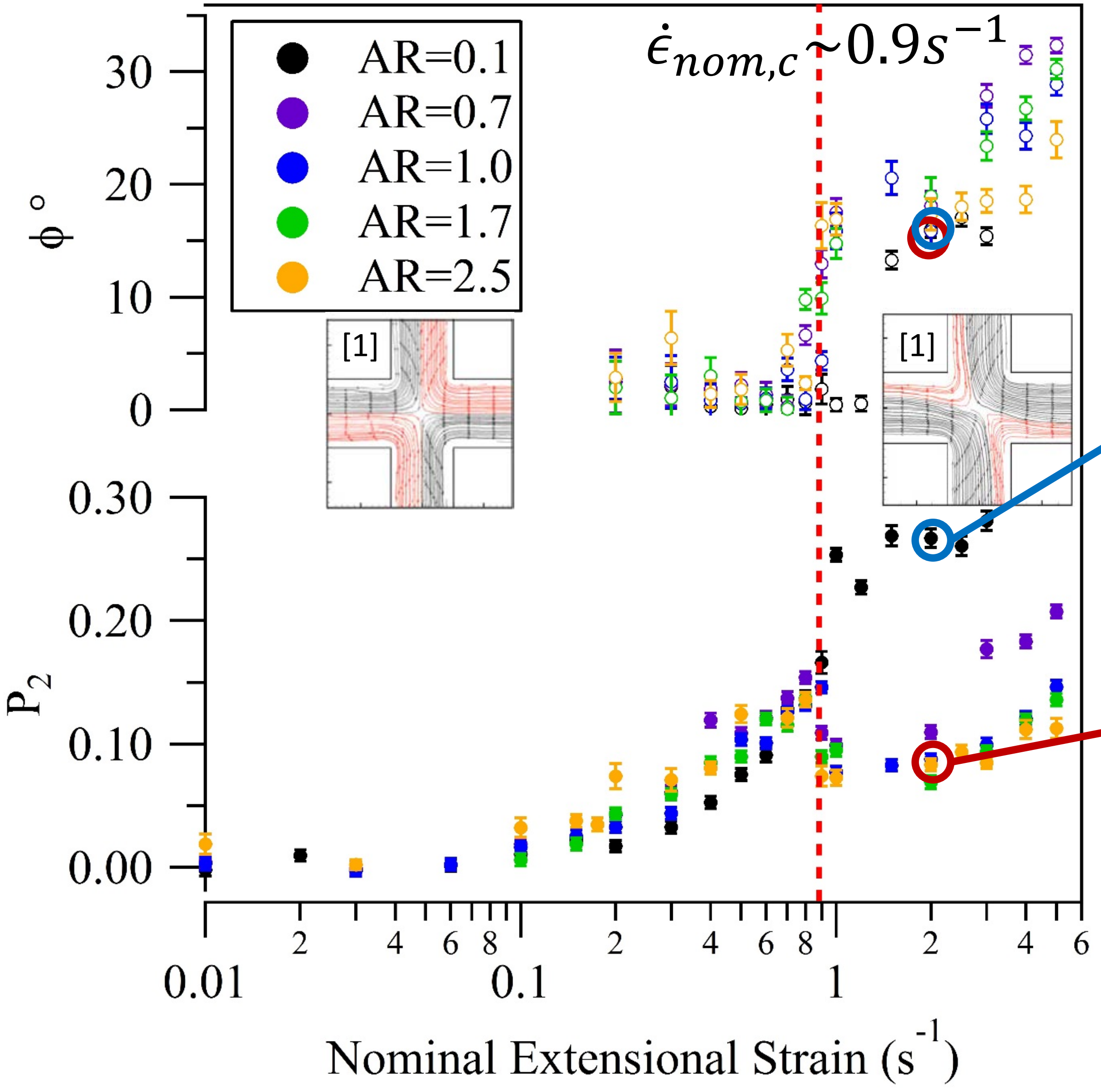


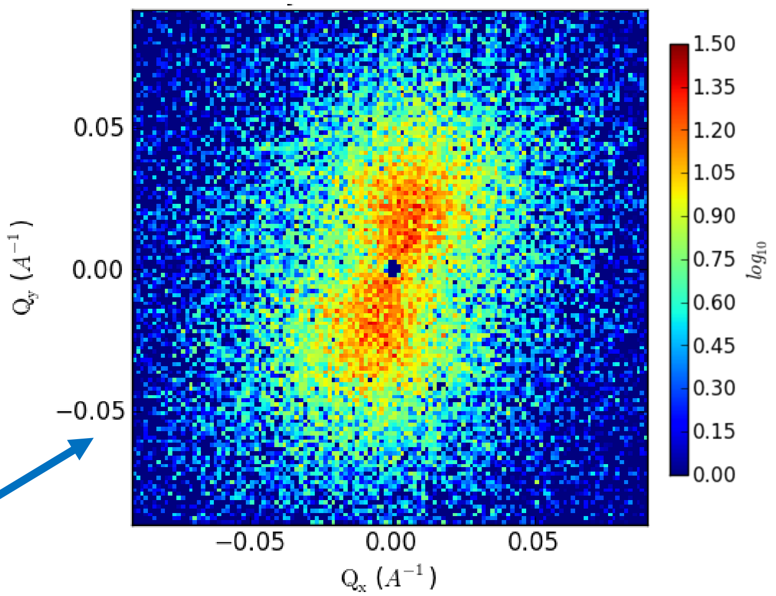
[1] Haward, S.; McKinley, G. *Physical Review.* **2012**, 85, 031502-1-031502-14

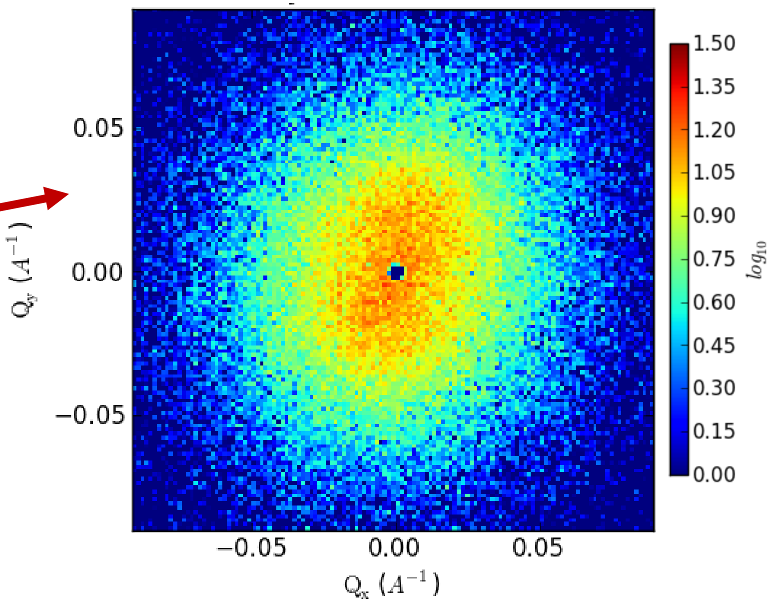
Orientation for Different Aspect Ratios

$\dot{\gamma}_{wall}$ is negligible

$$\dot{\epsilon}_{nom} = \frac{Q}{w^2 D}$$



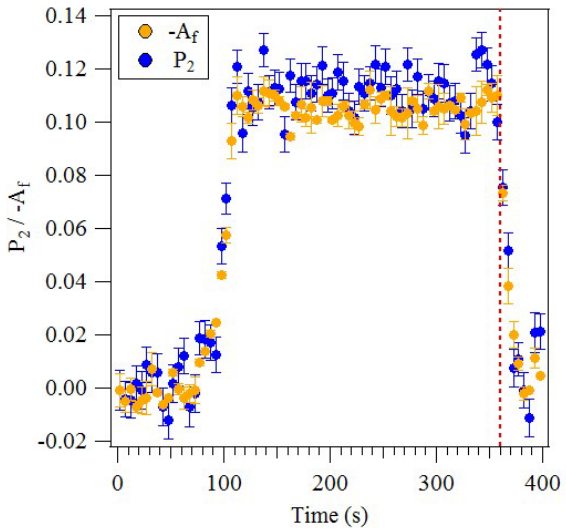


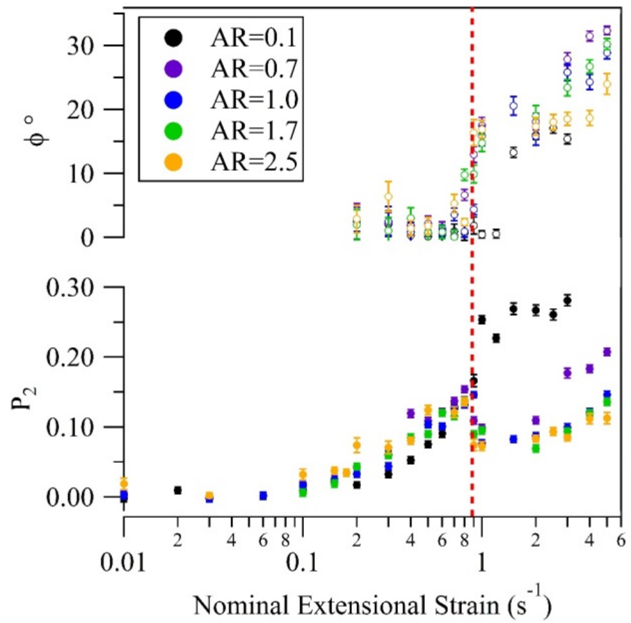


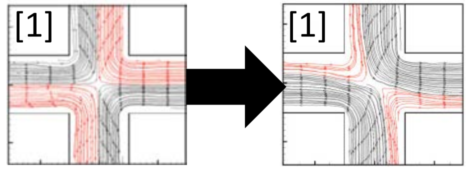
[1] Haward, S.; McKinley, G. *Physical Review.* **2012**, 85, 031502-1-031502-14

Conclusions

- $\bar{P}_2 \approx -A_f$
- Measured the amount of orientation and the angle of orientation as a function of nominal extensional strain rate
- Characterized the transition between symmetric and asymmetric flow
- Showed that the behavior of the higher aspect ratios is nearly identical

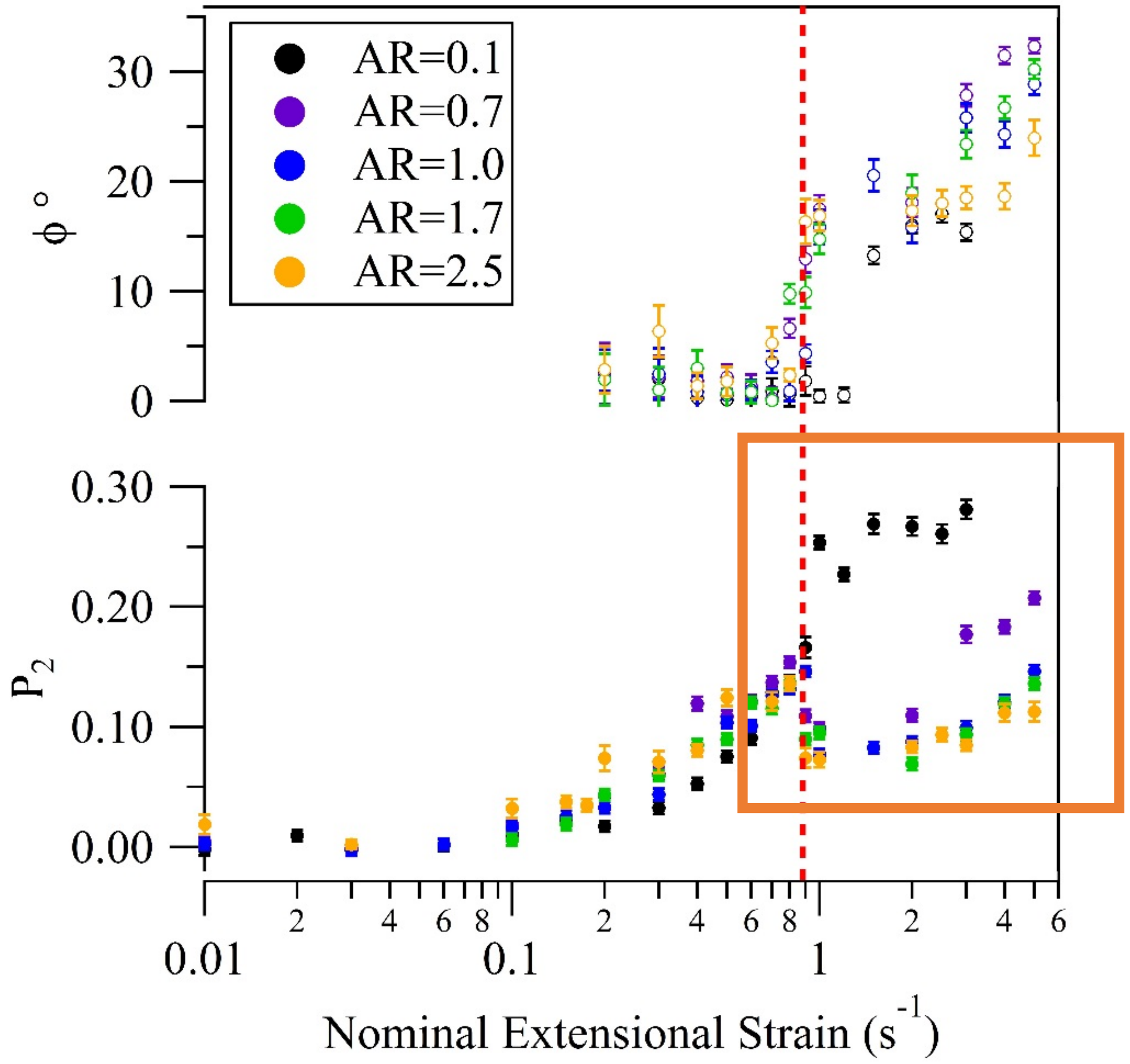


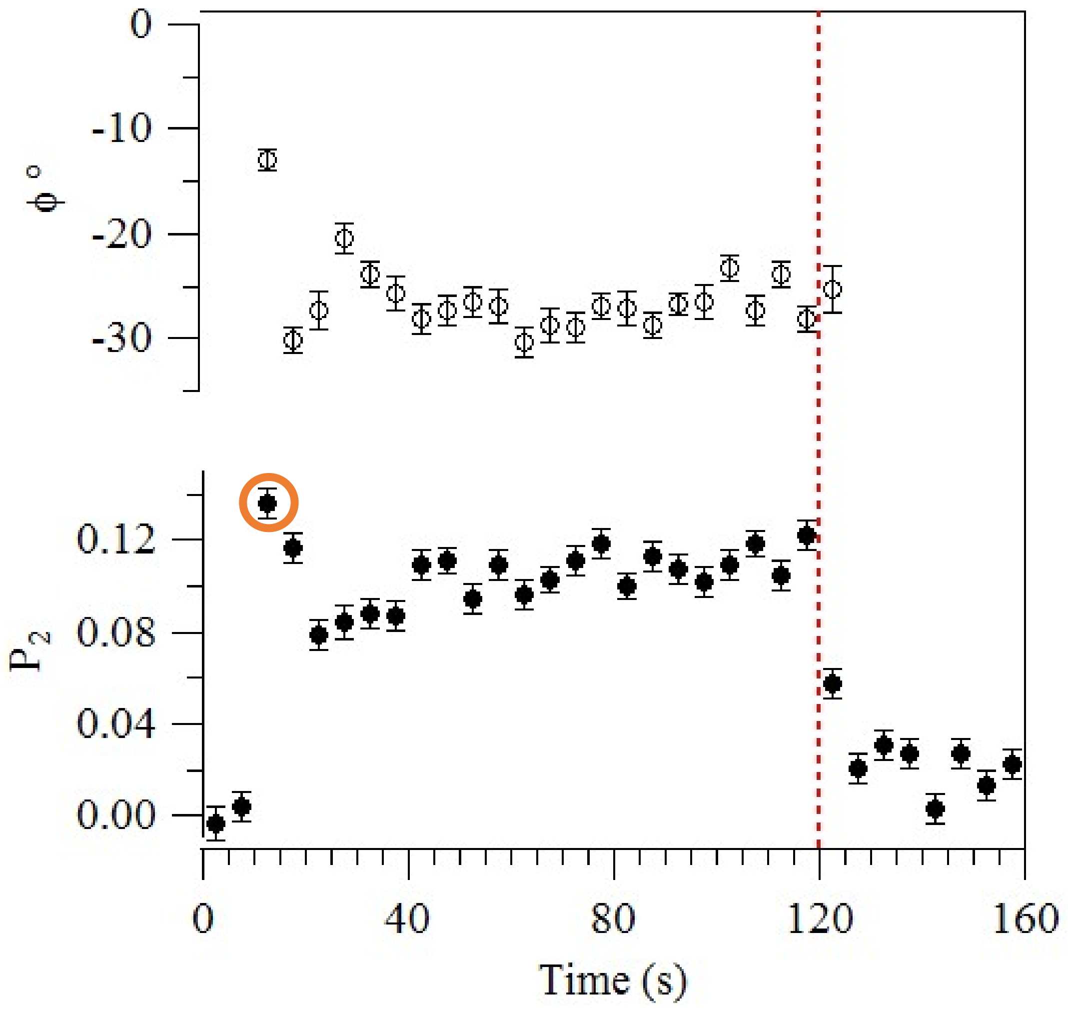




[1] Haward, S.; McKinley, G. *Physical Review.* **2012**, 85, 031502-1-031502-14

Future Work


AR=0.1
AR=0.7
AR=1.0
AR=1.7
AR=2.5
φ °
P2
0.01
0.1
1
Nominal Extensional Strain (s-1)


φ °
P2
Time (s)

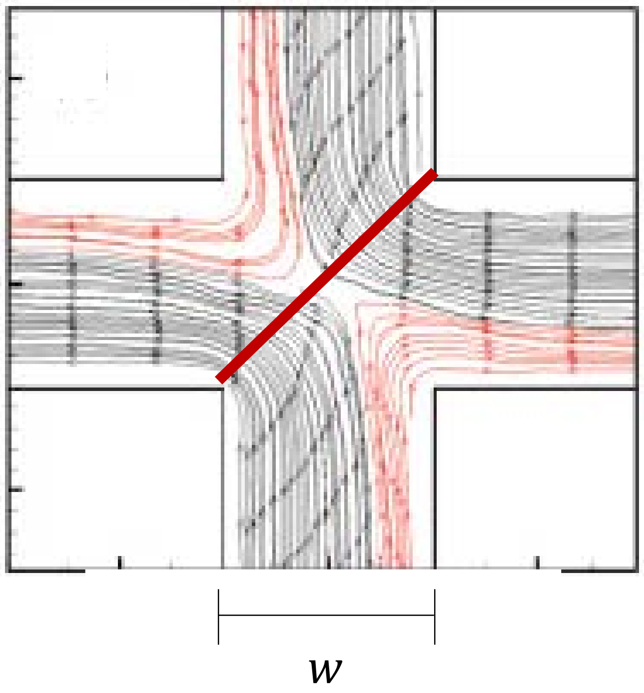
Acknowledgements

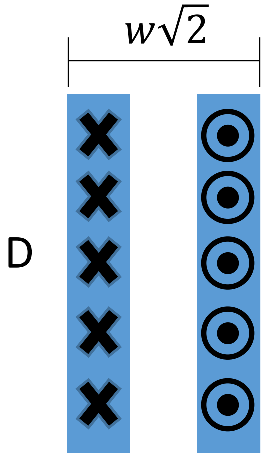
- Katie Weigandt
- NSF
- NIST- NCNR
- Julie Borchers
- David Hoogerheide, Chirag Parikh, and Frank Hess

Questions?

Aspect Ratio

$$AR = \frac{D}{w}$$

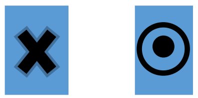




AR = 2.5

$$v = 8.5cm/s$$

$(\dot{\epsilon}_{nom} = 1s^{-1})$



AR = 1

$$v = 12cm/s$$

$(\dot{\epsilon}_{nom} = 1s^{-1})$

AR = .1

$$v = 42cm/s$$

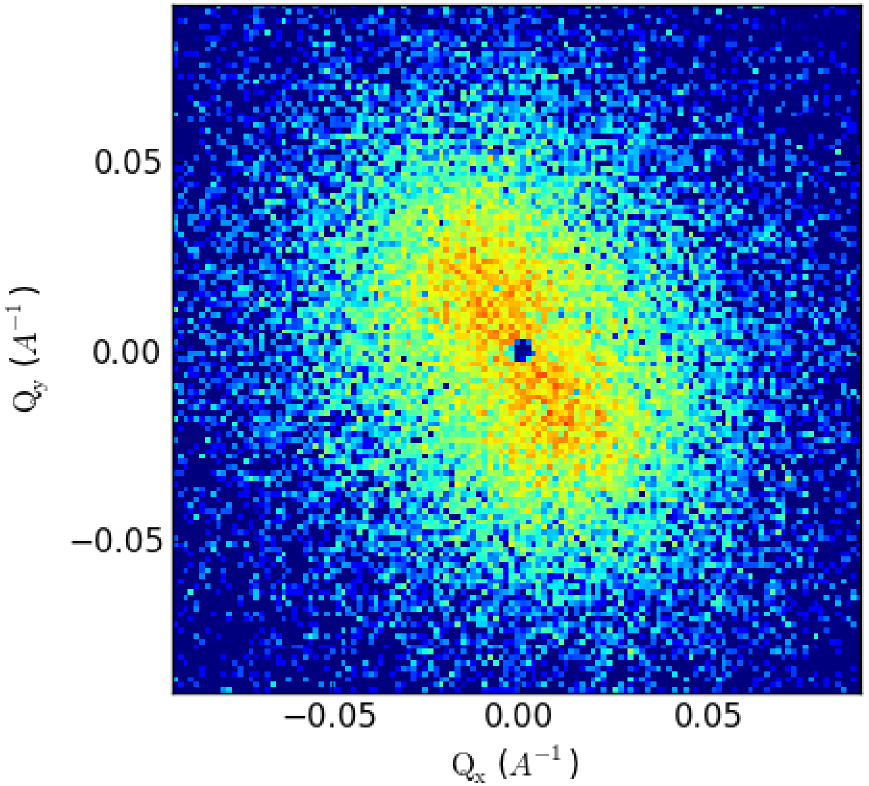
$(\dot{\epsilon}_{nom} = 1s^{-1})$

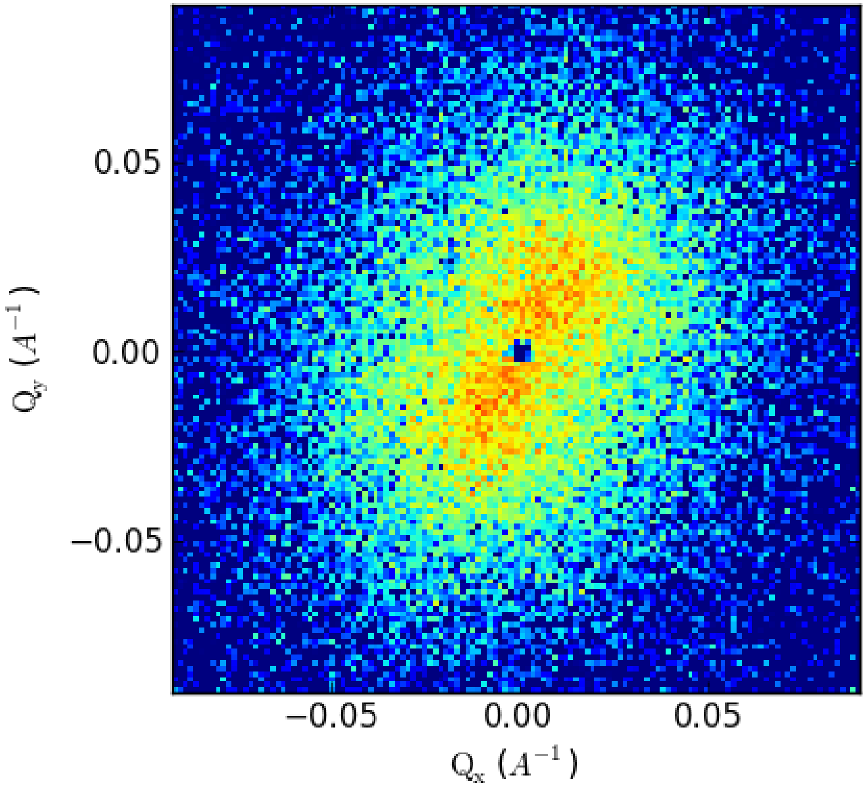
Plug-like flow:

$$\dot{\epsilon}_{nom} = \frac{Q}{w^2 D}$$ [1]

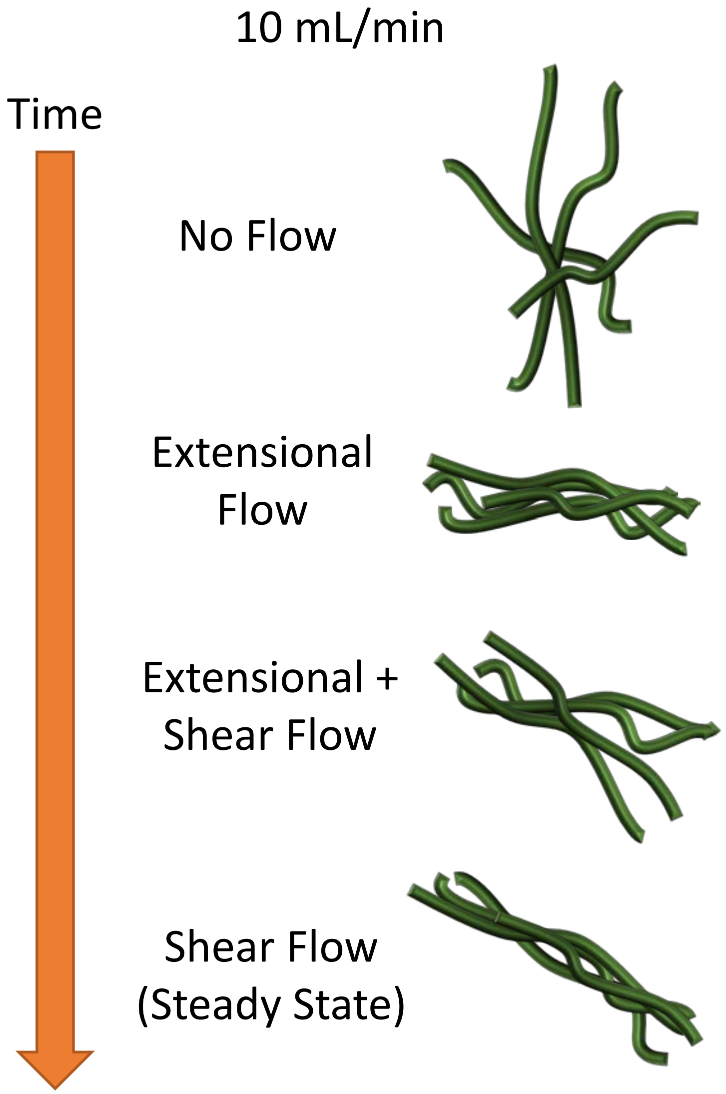
Preferential Asymmetry

$\dot{\epsilon} = 3s^{-1}$, AR = 0.7





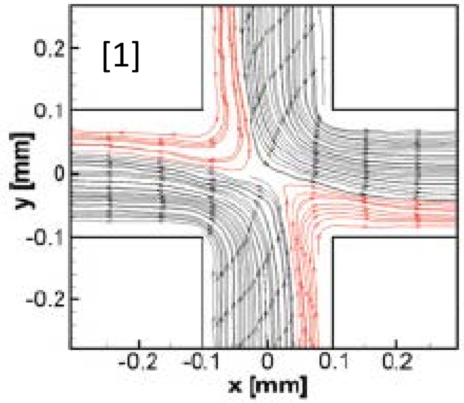
Stress overshoot

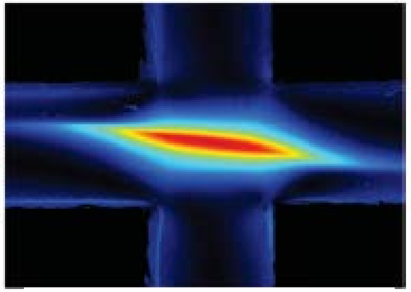


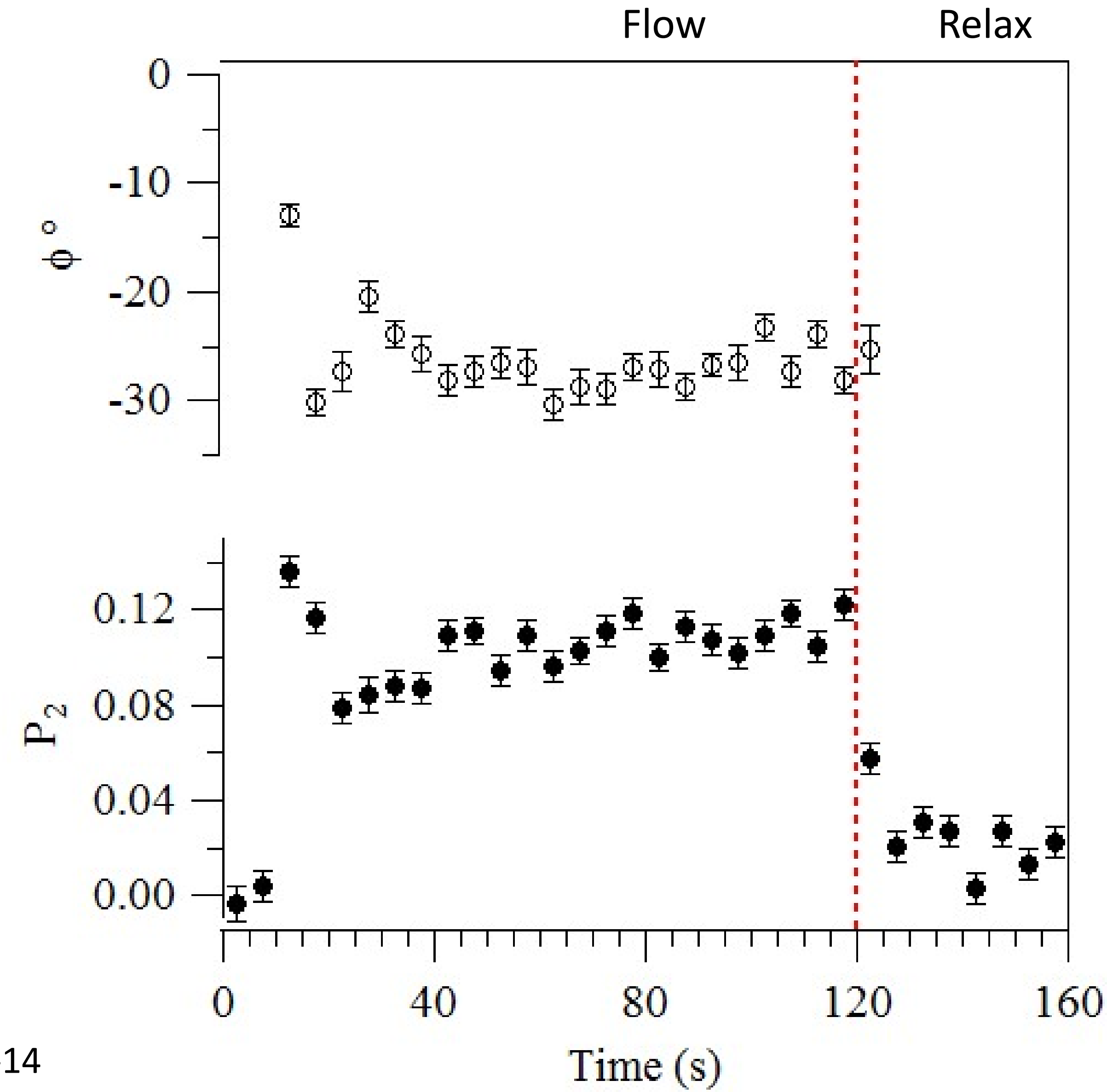
$\dot{\epsilon} = 8.3\ s^{-1}$ Time Resolved

Steady state orientation is reached after ~40s

$$\bar{P}_2 = 0.10$$
$$\phi_0 = -28°$$

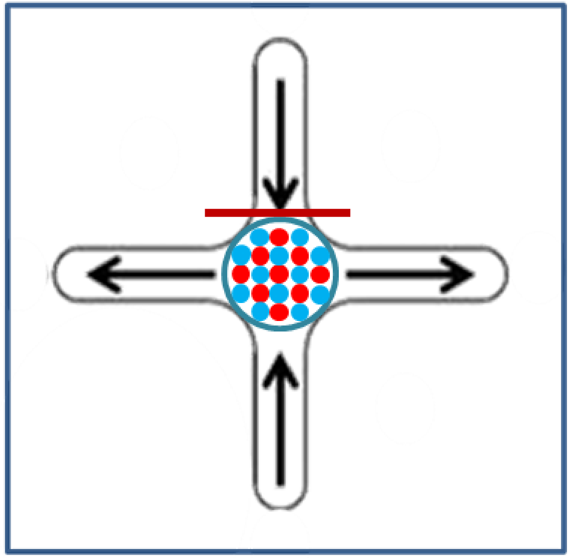


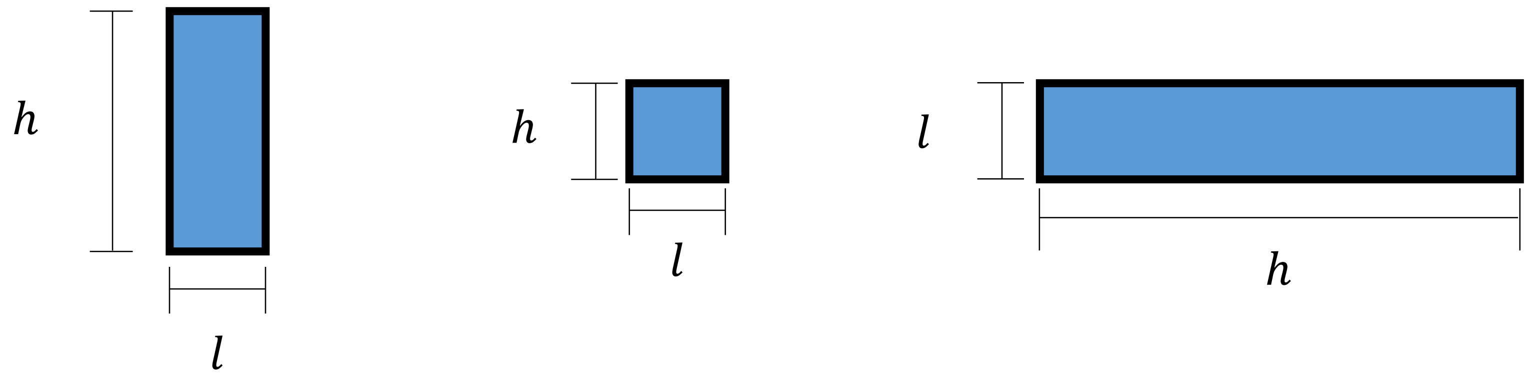




[1] Haward, S.; McKinley, G. *Physical Review.* **2012**, 85, 031502-1-031502-14

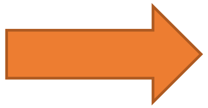
Aspect Ratios and Shear





$$\dot{\gamma}_{wall} = \frac{6Q}{l^2 h}; l < h$$ (Newtonian Fluid)

$$\dot{\epsilon}_{nom} = \frac{Q}{w^2 D} = 1\, s^{-1}$$



$\dot{\gamma} = 6\, s^{-1}$ $\dot{\gamma} = 6\, s^{-1}$ $\dot{\gamma} = 36.8\, s^{-1}$

Symmetric Flow

References

1. Haward, S.; McKinley, G. *Physical Review.* **2012**, 85, 031502-1-031502-14
2. W. H. DeJeu, *Mol. Cryst. Liq. Cryst*. **1997,** 292, 13.
3. L.M. Walker, “Rheology and Rheo-optics of liquid crystal polymers under flow.” **1995**