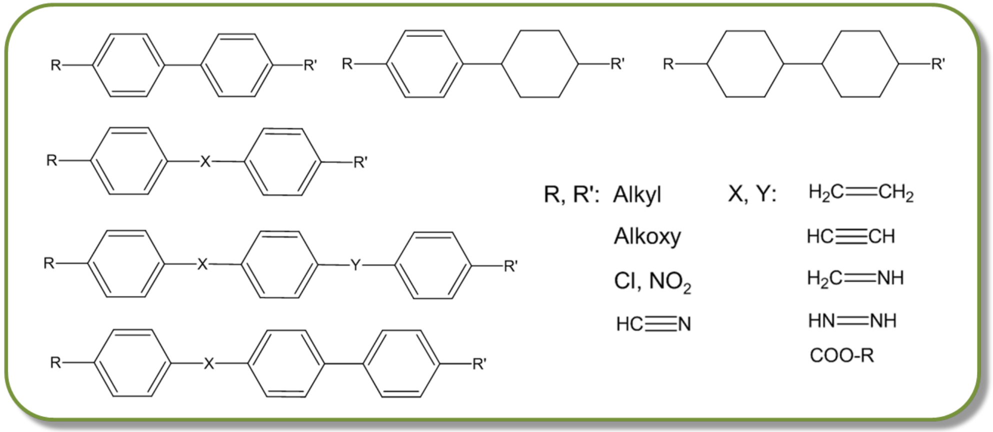
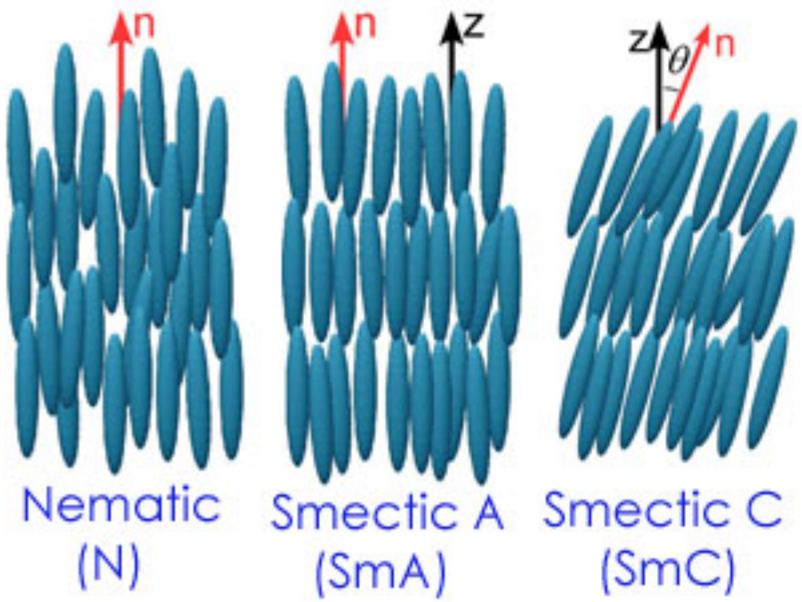
Dynamics of sheared liquid crystals

Liquid crystalline materials

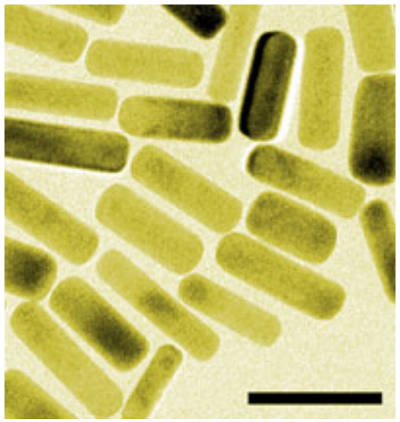
mesogenic molecules
(thermotropic liquid crystal)

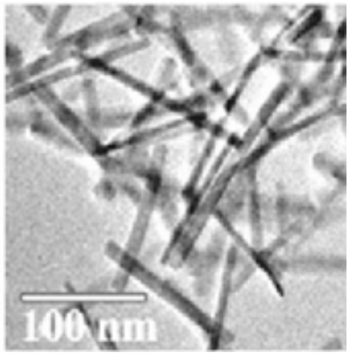


formation of mesophases
(nematic, smectic, ….)

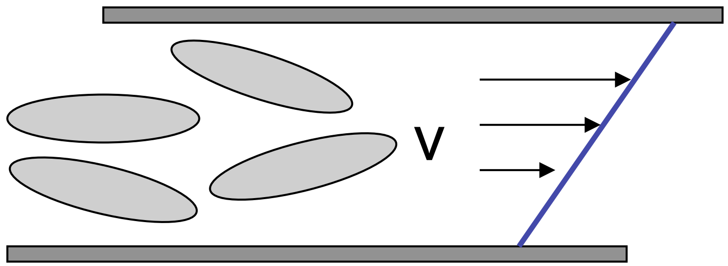


colloidal nanorods





Behavior under shear ?



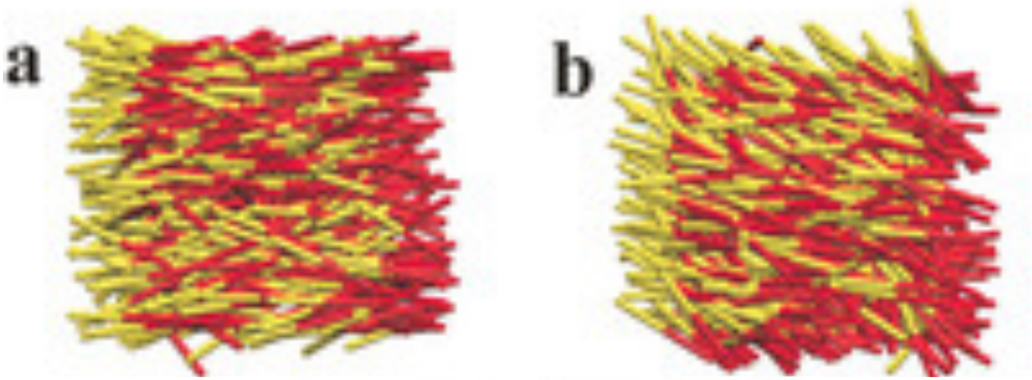
planar Couette flow

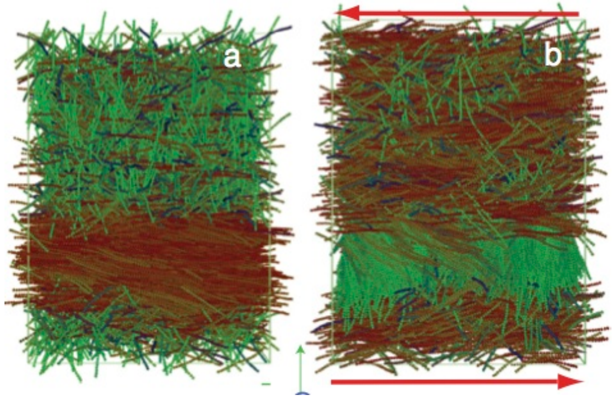
Complex orientational dynamics (stationary and oscillatory states, spatial symmetry breaking, …..)

Applications:
Rheology (material science), particles in blood flow, ….

Shear-induced dynamics on the particle level

Computer simulations



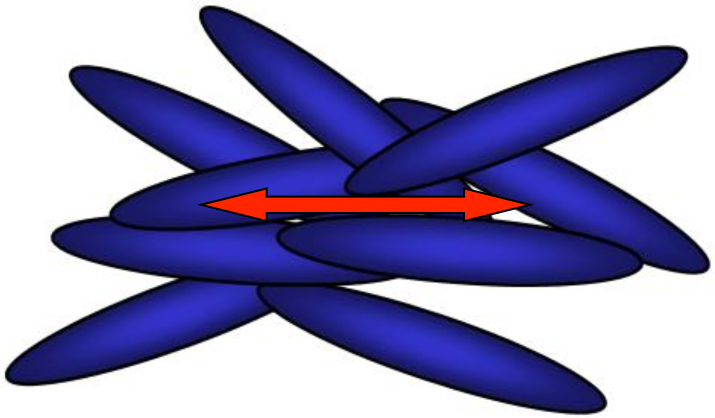


W.J. Briels, Twente
M. Ripoll, G. Gompper, Juelich

Experiments

P. Lettinga, J. Dhont, Jülich

mesoscopic description of the orientational dynamics



$\underline{\underline{Q}}(\underline{r},t)$

tensorial order parameter
(5 independent components)

- director dynamics
- biaxiality
- dynamic behavior in and out of the shear plane

Orientational dynamics on the mesoscopic level

Equation of motion for the alignment tensor
(homogeneous system, i.e., infinite plate separation)

$$\frac{d}{dt}\underline{\underline{Q}} - 2\overline{\Omega \times \underline{\underline{Q}}} + \frac{\partial \Phi^{LG}}{\partial \underline{\underline{Q}}} = \sqrt{\frac{3}{2}}\lambda_K \overline{\nabla \underline{v}}$$

$$\lambda_k \sim \frac{q^2 - 1}{q^2 + 1}$$

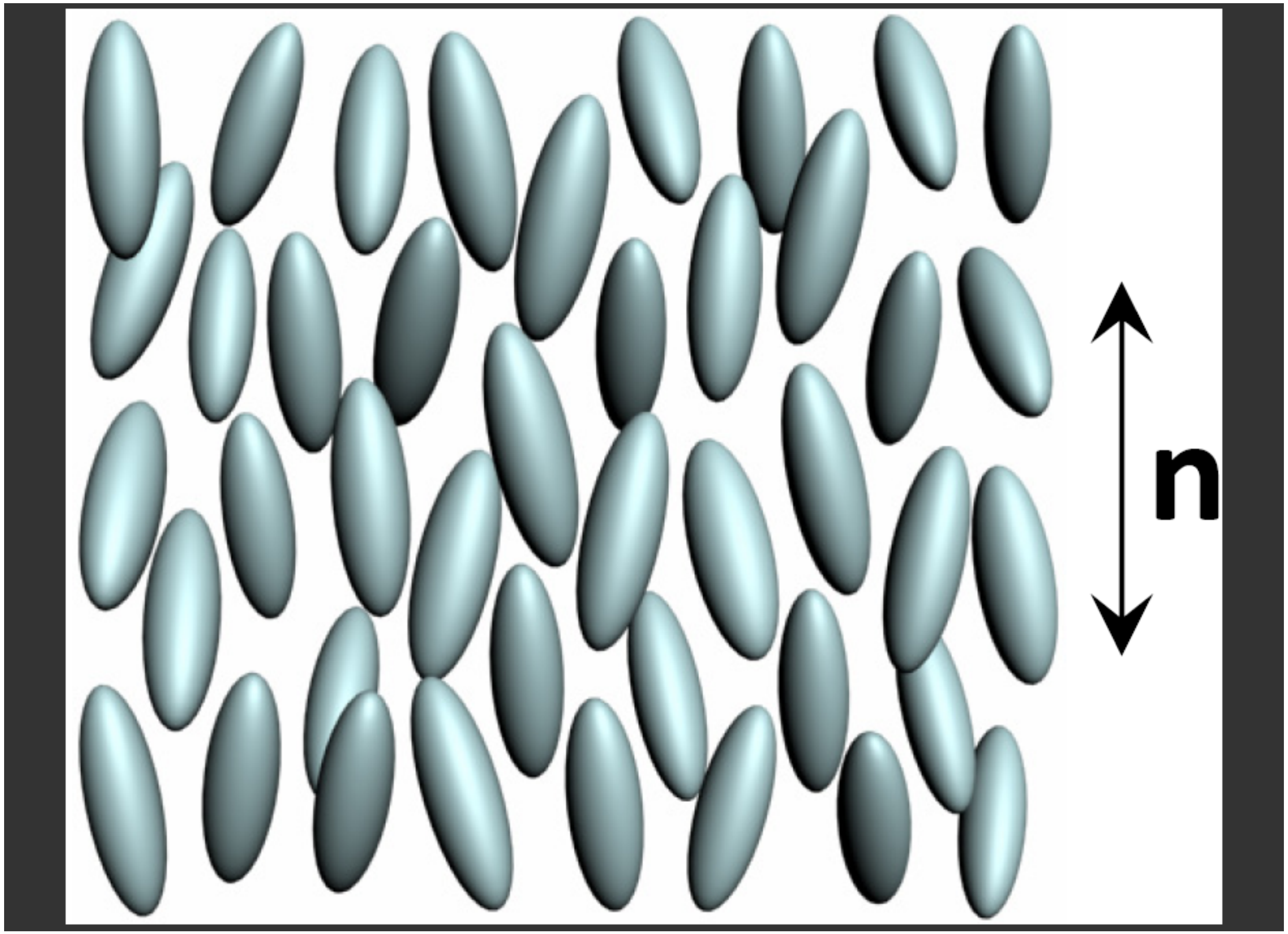
coupling to shear flow
with velocity field $\underline{v}$

relaxational term: Φ^{LG} Landau-de Gennes free energy

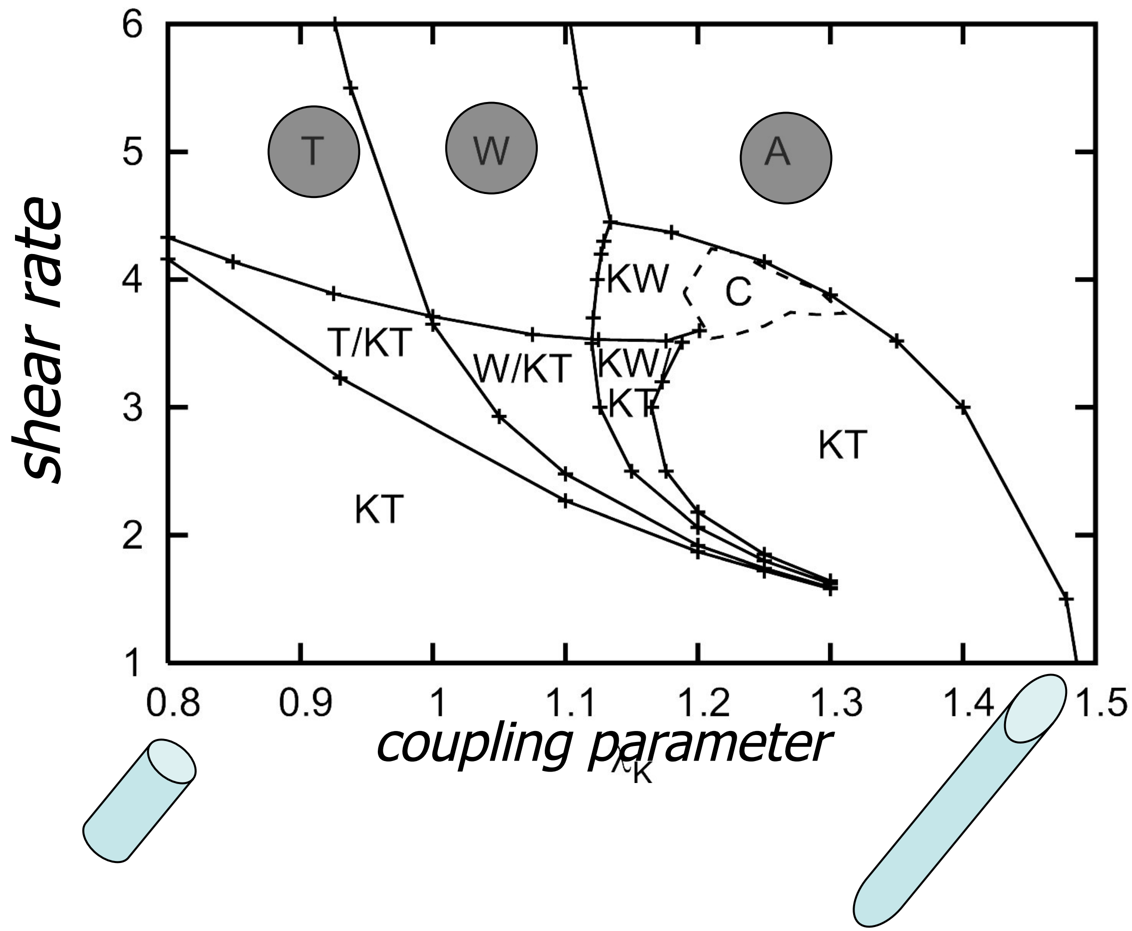
→ 5-dimensional system

S Hess, Z. Naturforschung 1975, M Doi, Ferroelectrics 1980
S Grandner, S Heidenreich, S Hess, SHL Klapp, Eur Phys J E 2007

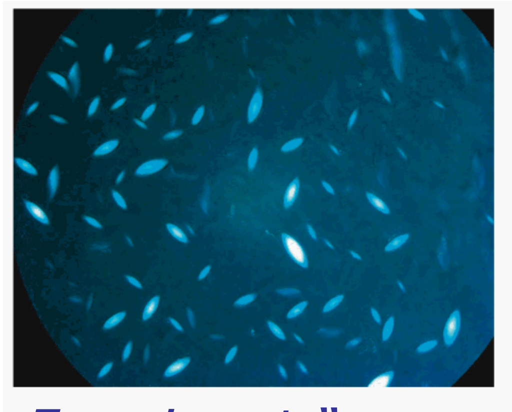
Shearing the system starting from a nematic state ...



Homogeneous systems: Dynamic „phase“ diagram



$$\lambda_k \sim \frac{q^2 - 1}{q^2 + 1}$$

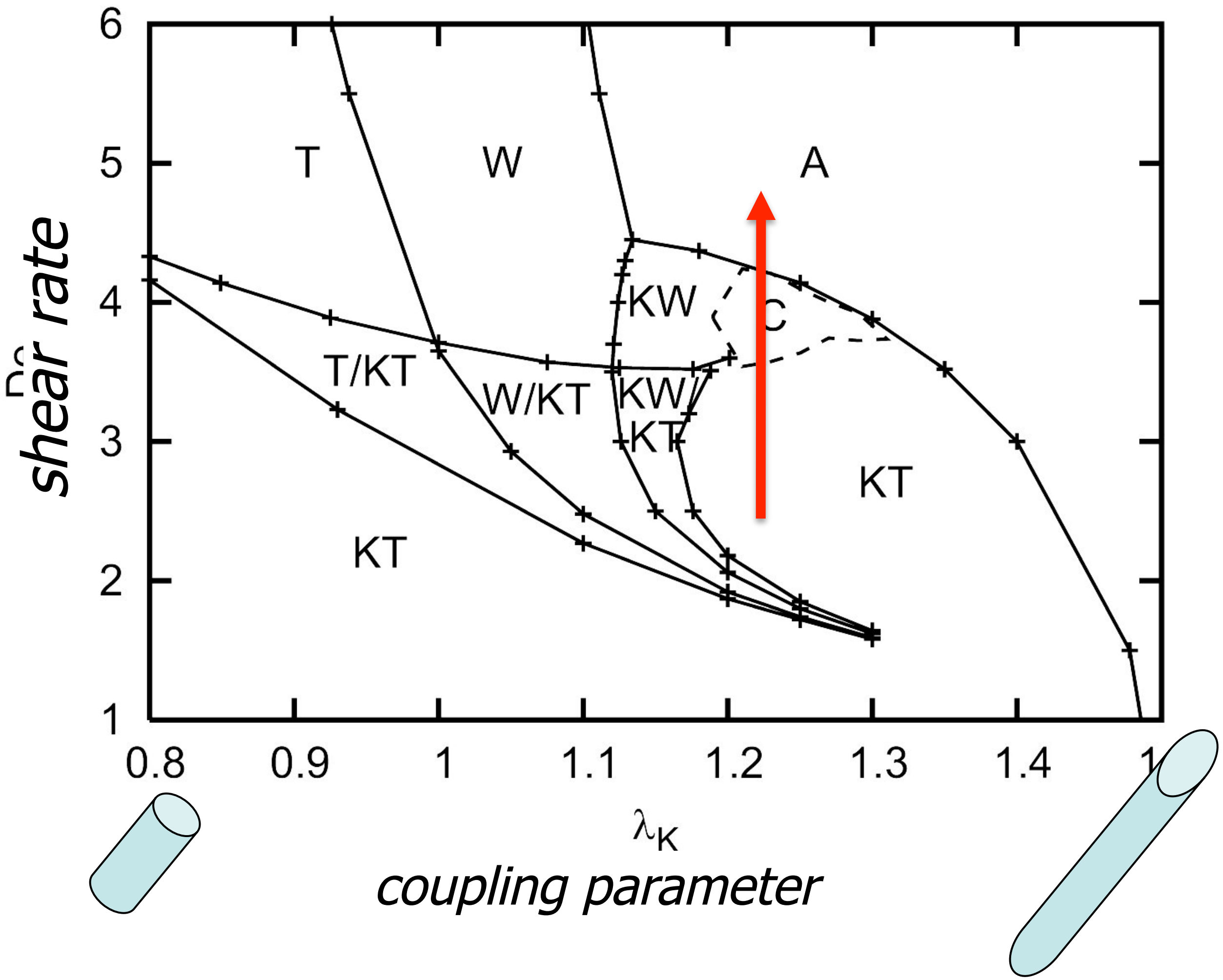


Experiments“:
P. Lettinga, J. Dhont, Jülich

G. Rienaecker, M. Kroeger, S. Hess, Phys Rev E(R) 2002,
S Grandner, S Heidenreich, S Hess, SHL Klapp, Eur Phys J E ***24****, 353 (2007)*

Rheology?

Consider systems with fixed coupling parameter λ_K
(i.e. particles with fixed shape)

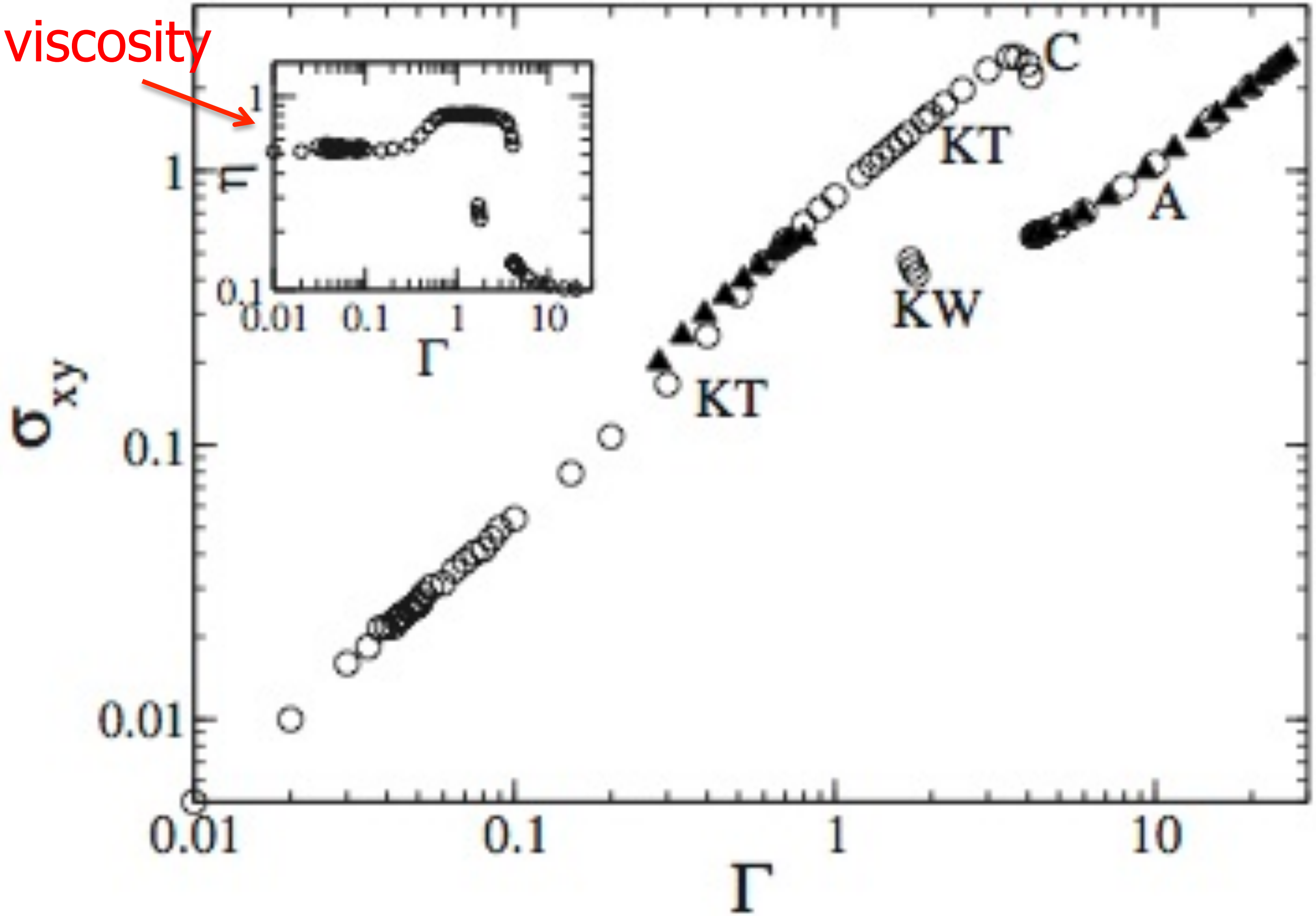


A:
„shear alignment"
(stationary)

C:
„complex"
(irregular)

KT:
„kayaking-tumbling"
(oscillatory)

Shear stress versus shear rate



S.H.L. Klapp, S. Hess, Phys. Rev. E **81**,051711 (2010)

boundary effects

*S Heidenreich, S Hess, SHL Klapp, Phys Rev Lett **102**, 028301 (2009)*

Extension towards surface effects

1) Ginzburg-Landau free energy for the equilibrium part

$$g(\underline{d},\underline{\underline{Q}}) = \frac{k_B T}{m}\Big(\Phi^Q + \Phi^d + \Phi^{Qd} + \frac{\xi_Q^2}{2}\nabla\underline{\underline{Q}} : \nabla\underline{\underline{Q}} + \frac{\xi_d^2}{2}\nabla\underline{d} : \nabla\underline{d} - c_f(\underline{d}\nabla) : \underline{\underline{Q}}\Big)$$

homogeneous parts

2) interplay flow ⟺ orientational motion

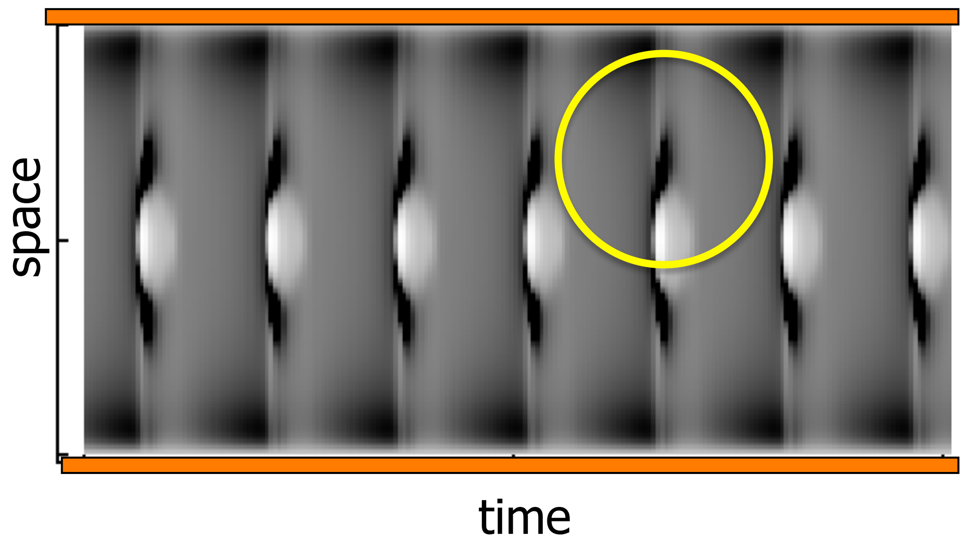
$$\frac{\mathrm{d}}{\mathrm{dt}}\underline{\mathrm{v}} = -\mathrm{k_B T}\,\nabla\underline{\underline{\mathrm{P}}}$$

pressure tensor

$$\underline{\underline{\mathrm{P}}} = -2\eta_{\mathrm{iso}}\nabla\underline{\mathrm{v}} + c\Big(\Phi^Q - \xi_Q^2\Delta\underline{\underline{\mathrm{Q}}} + c_f\nabla\underline{\mathrm{d}} + \frac{c_0}{2}\underline{\mathrm{d}}\,\underline{\mathrm{d}}\Big)$$

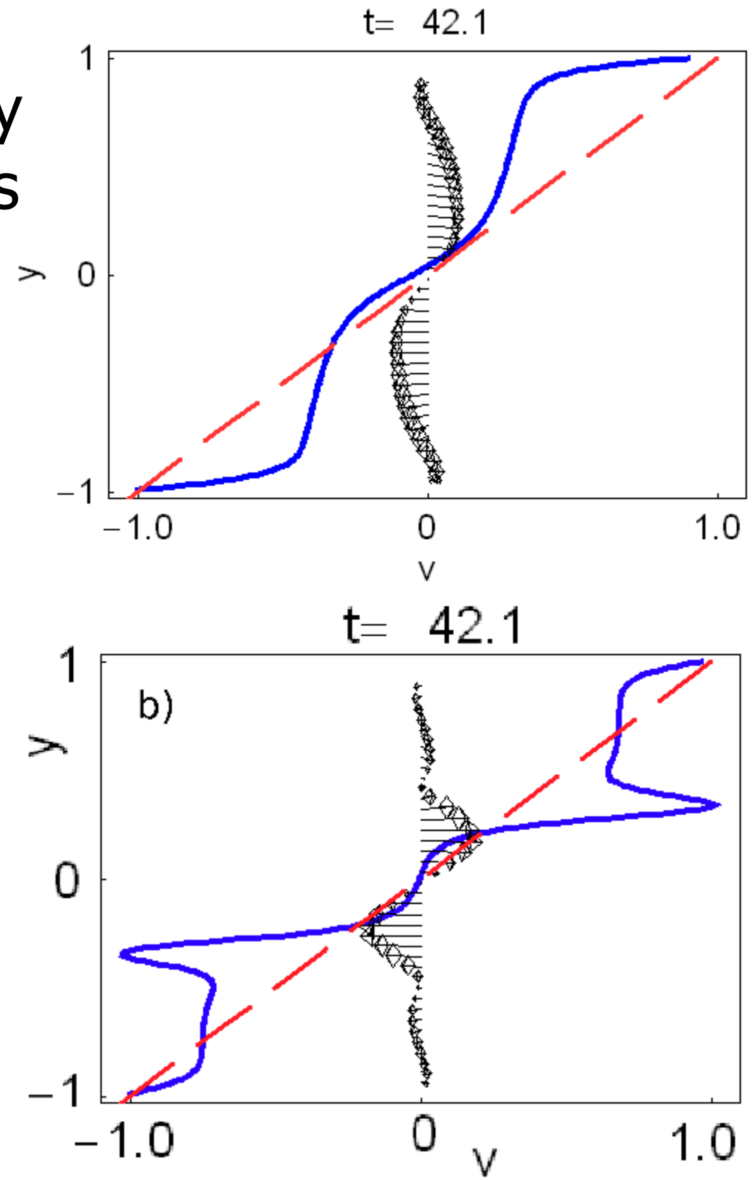
feedback mechanism!

Inhomogeneous systems: director dynamics

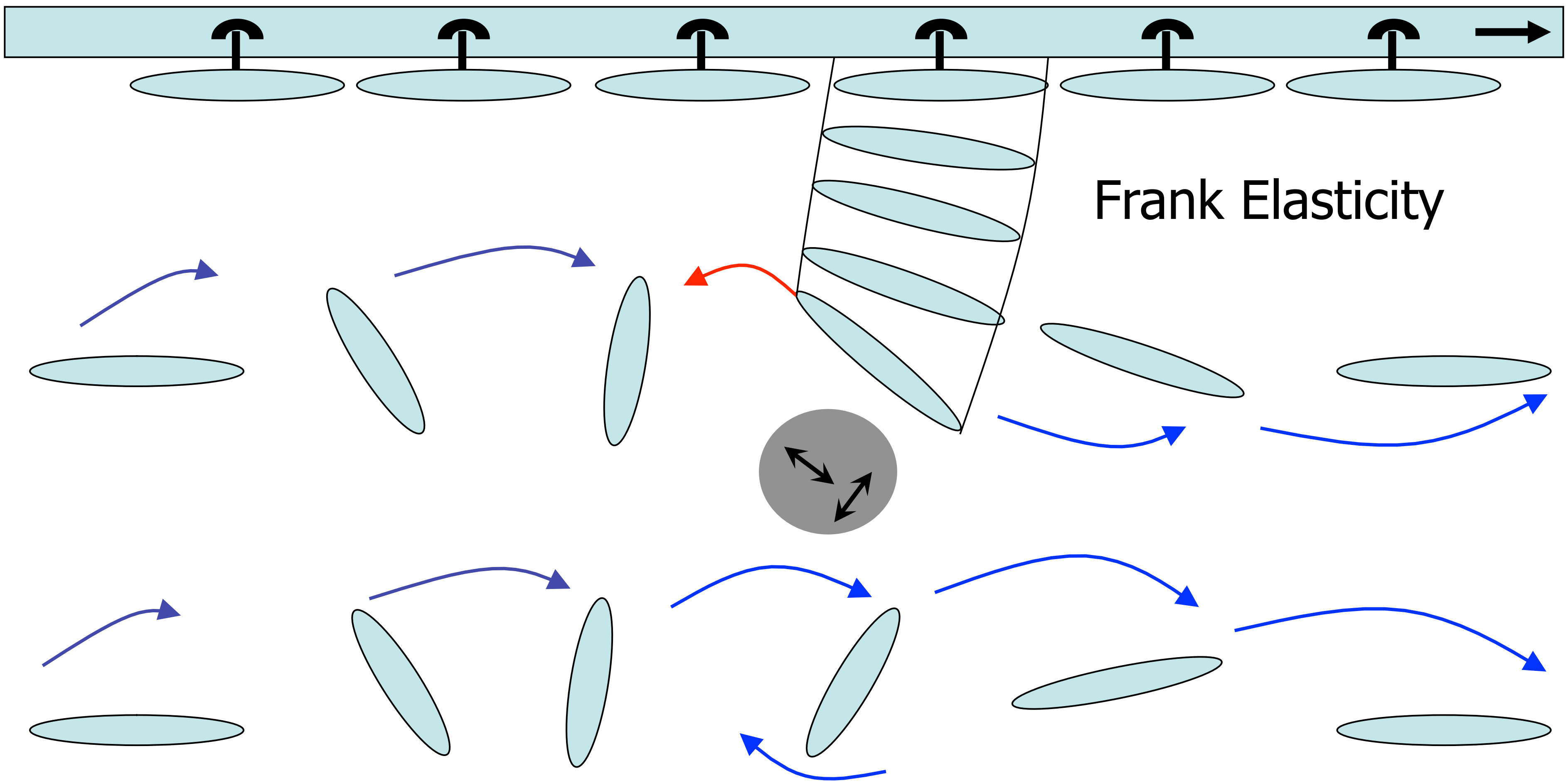


largest eigenvalue of $\underline{Q}(\underline{r},t)$

velocity profiles



Director analysis

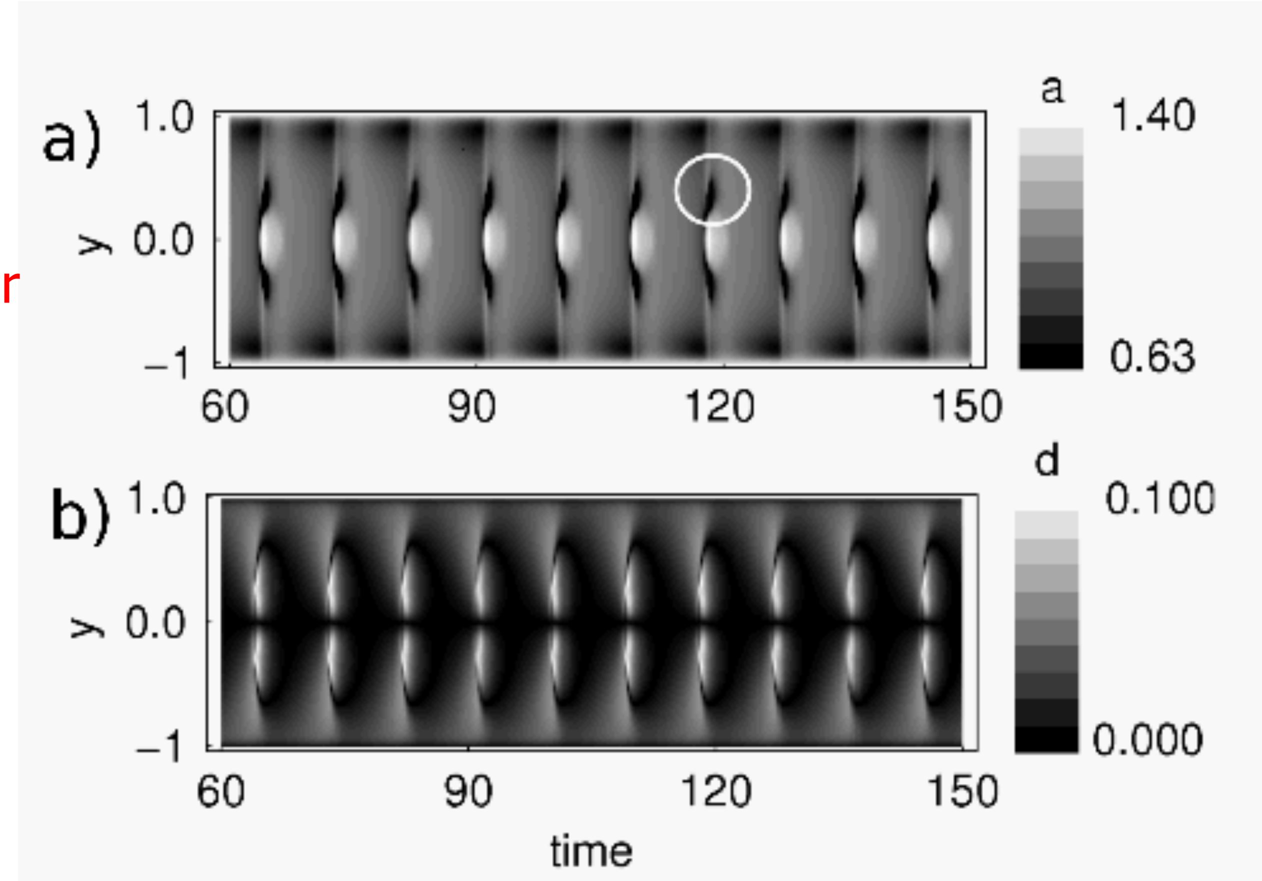


Competition between tumbling and wagging !

Dynamics of the dipole moment

director

dipole



shear-induced time-dependent polarization!

*S Heidenreich, S Hess, SHL Klapp, Phys Rev Lett **102**, 028301 (2009)*