

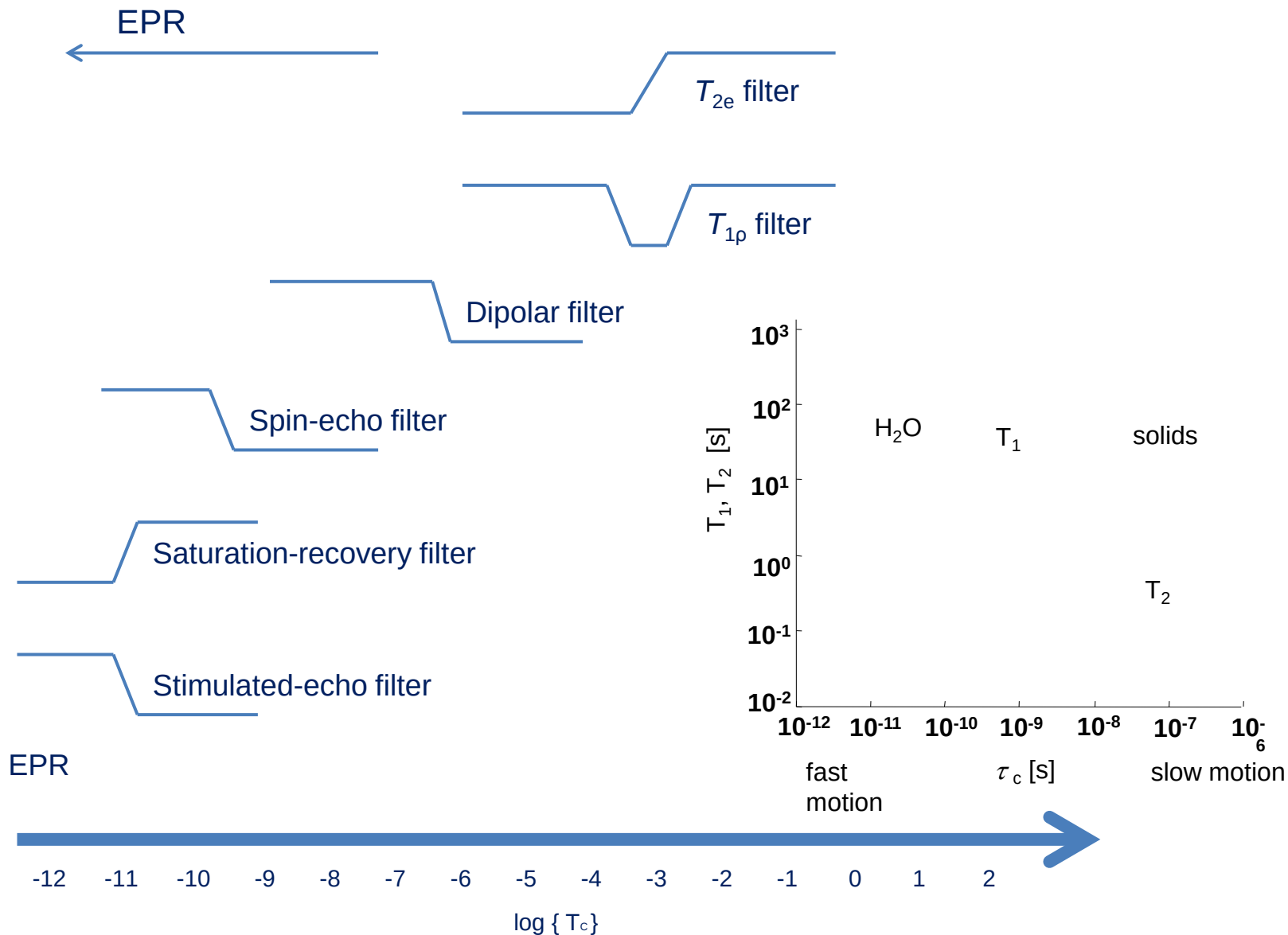
Stability and molecular mobility for phase-change materials

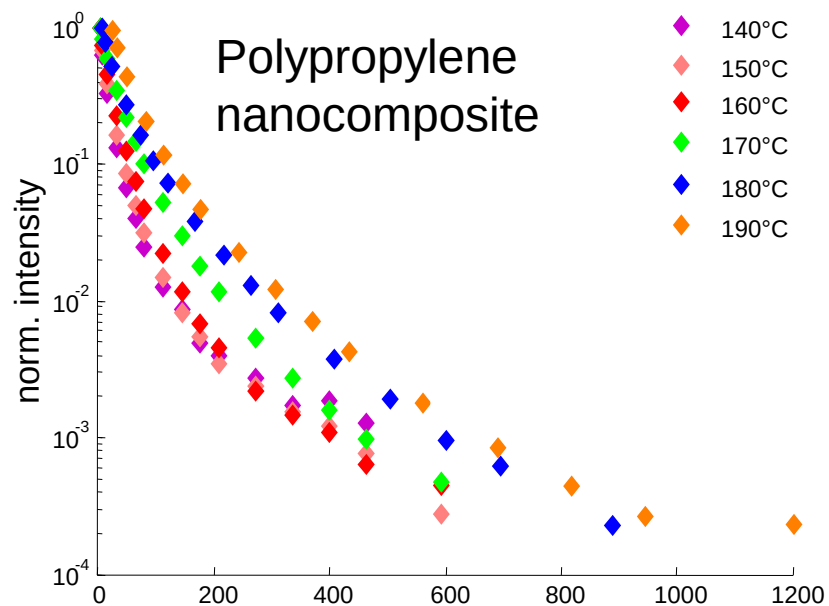
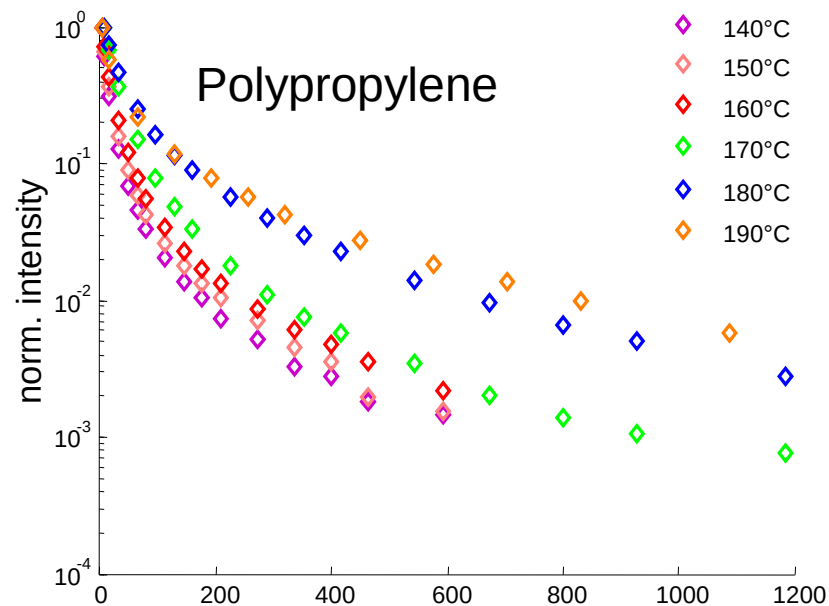
Ulrich Scheler

Leibniz-Institut für Polymerforschung Dresden e.V.

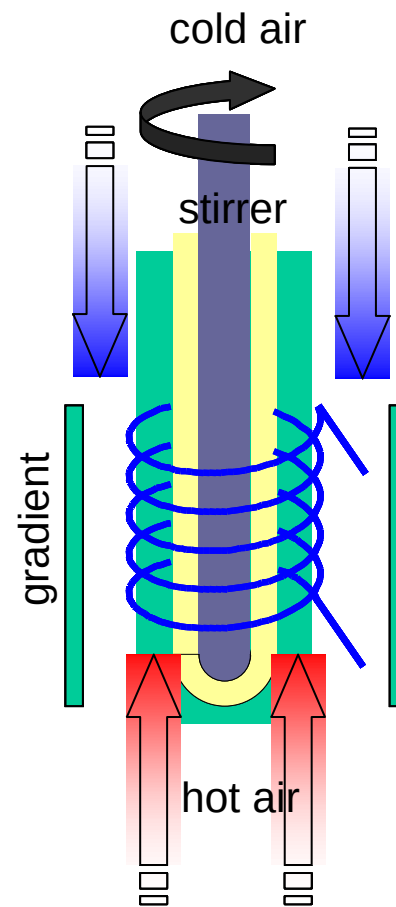
scheler@ipfdd.de

www.ipfdd.de



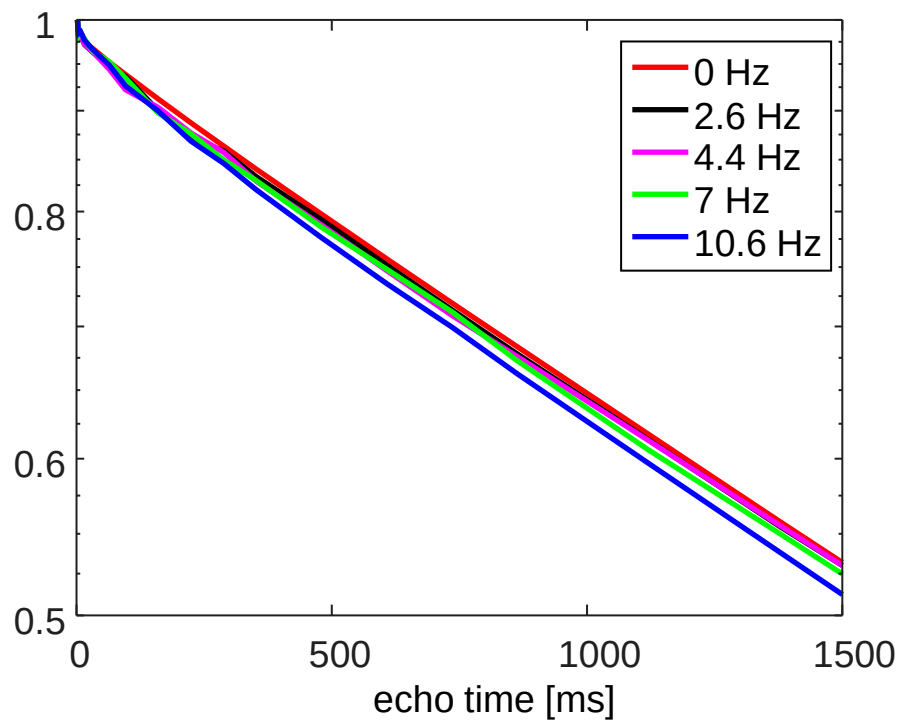


High-temperature Rheo NMR

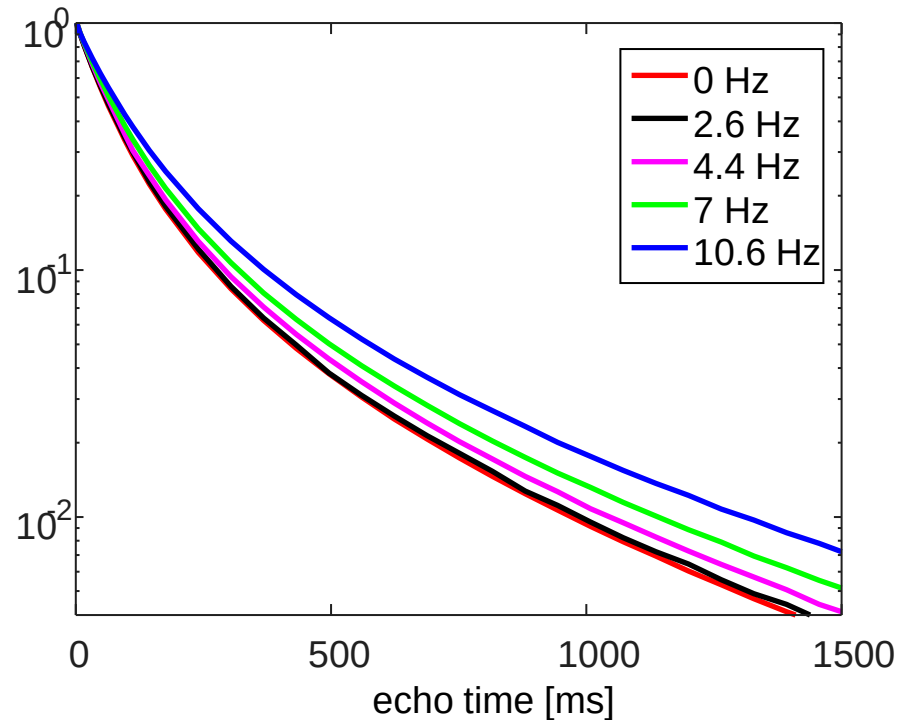


U.Böhme, U. Scheler, NMR Spectroscopy of Polymers: Innovative Strategies for Complex Macromolecules, Cheng, H.N.; Asakura, T.; English, A.D., ed. (ACS Publisher 2011) 1077, Chapter 26

0.4 kg/mol

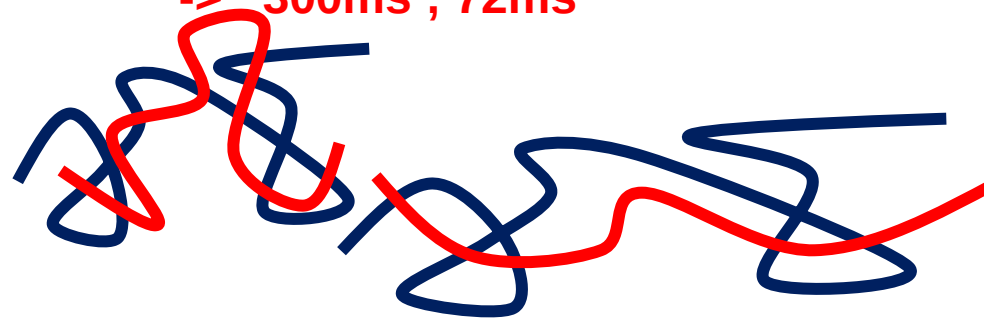


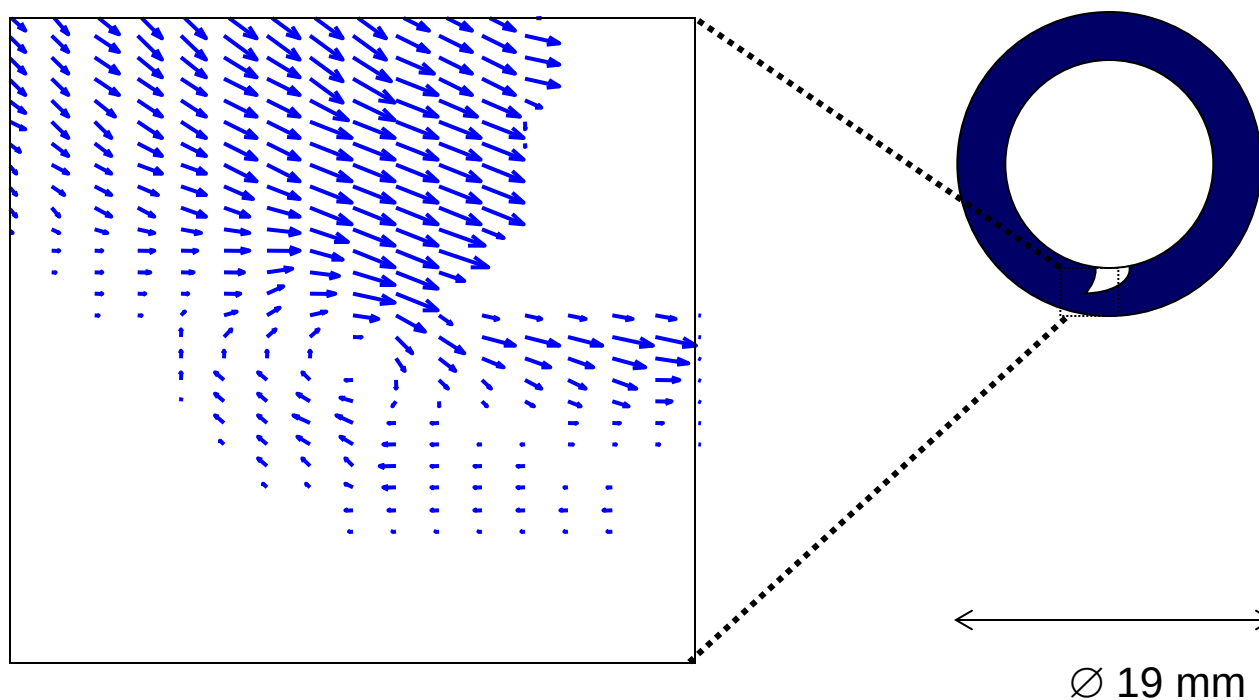
630kg/mol



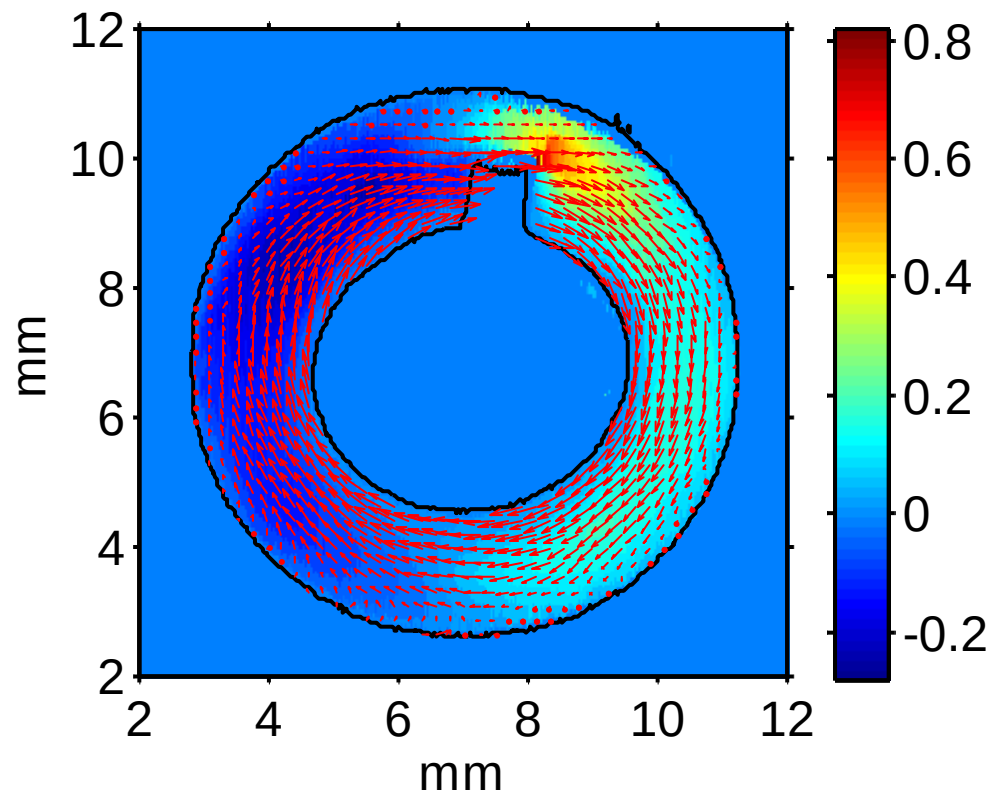
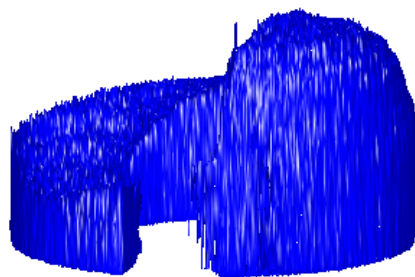
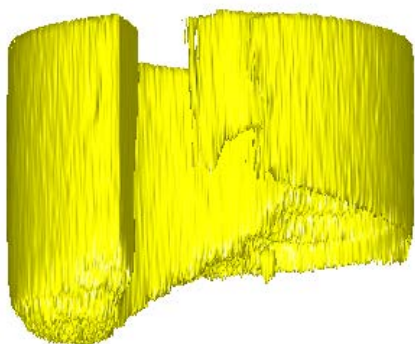
$T_2 = 1800\text{ms} \rightarrow 1650\text{ms}$

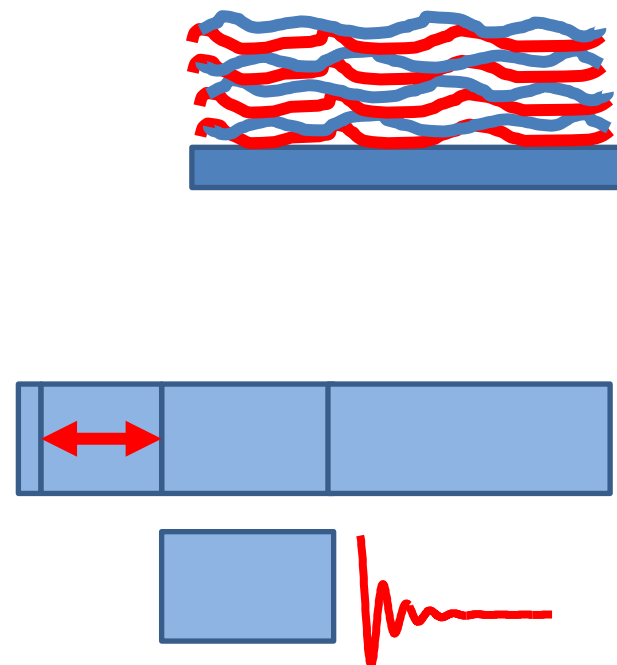
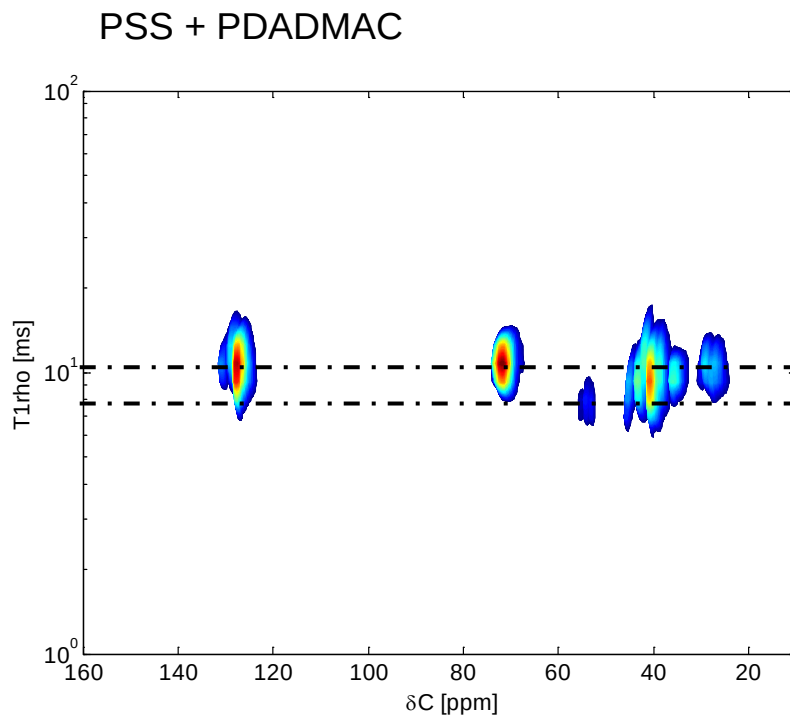
$T_2 = 250\text{ms} ; 60\text{ms}$
 $\rightarrow 300\text{ms} ; 72\text{ms}$





under rotation



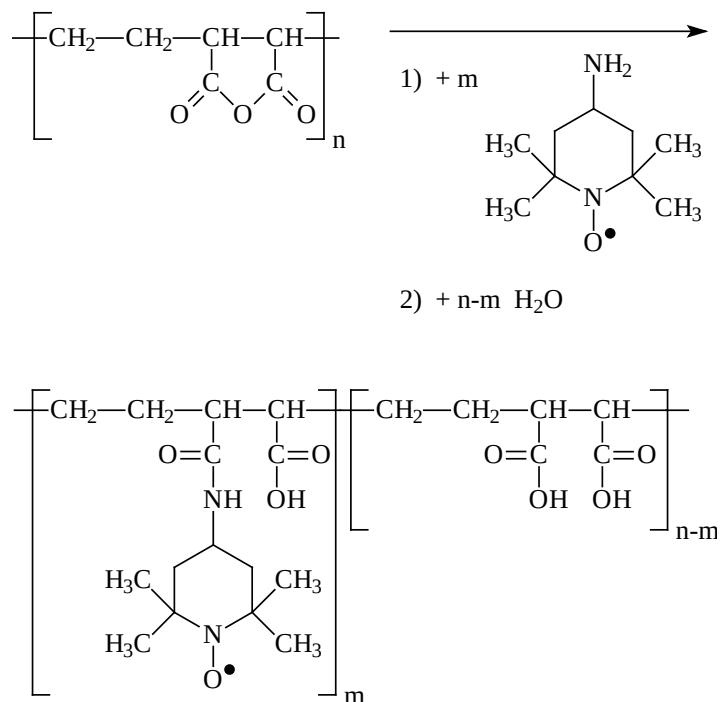


F2: FT $\rightarrow$ CS
F1: ILT $\rightarrow T_{1\rho}$

Poly(ethylene-*alt*-maleic acid)

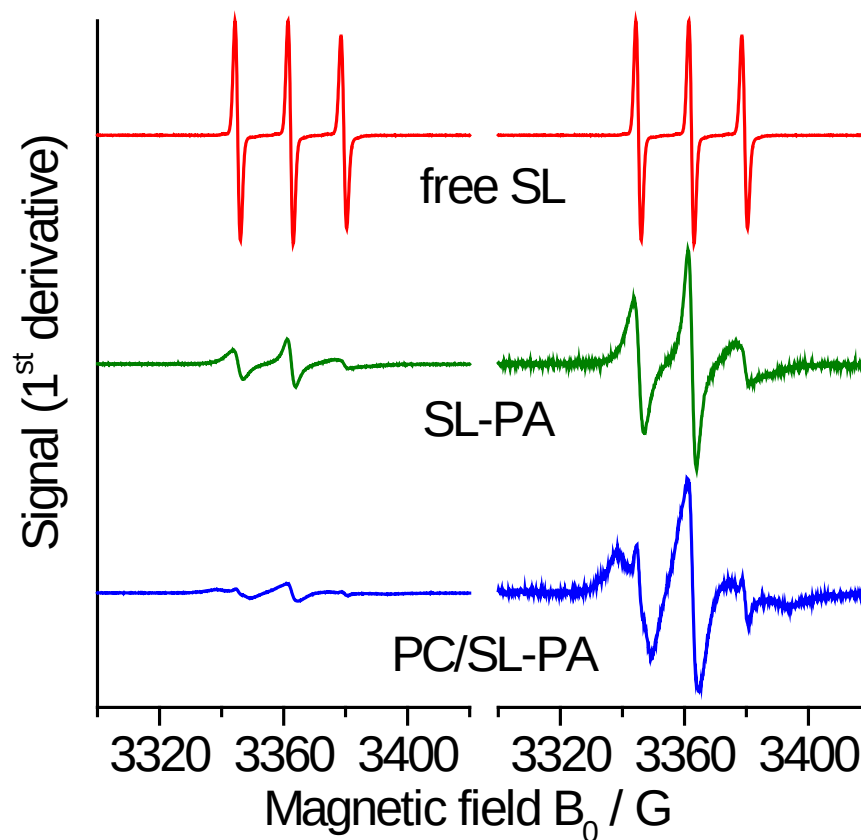
P(E-*alt*-MA)

- one spin label per ~40 repeat units

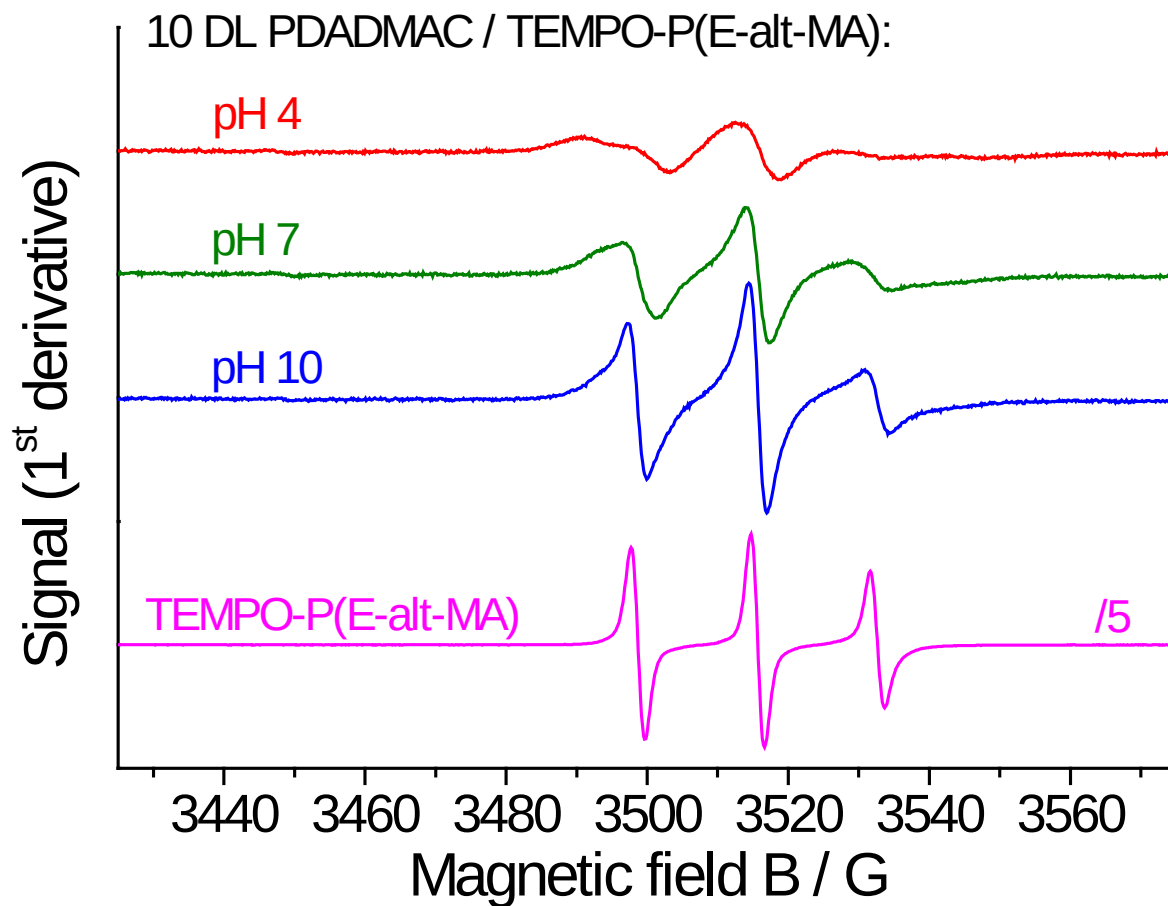
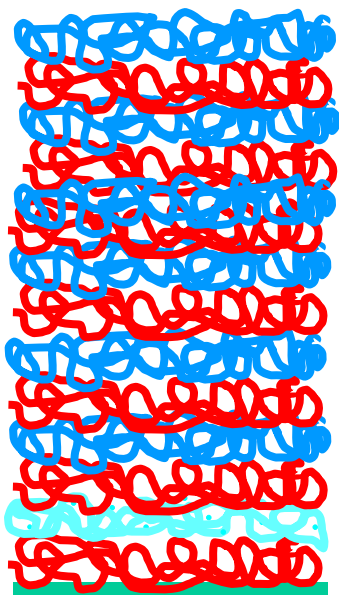


CW EPR spectra (X-band)
in aqueous solution

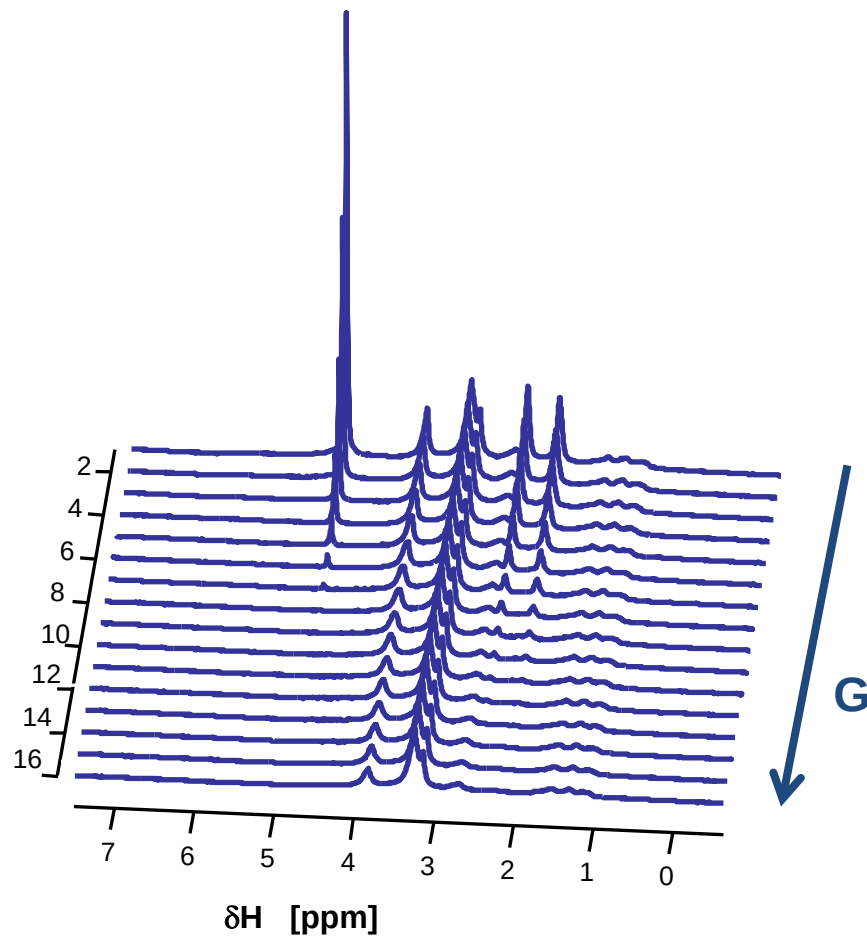
Coupling of the free electron with the
¹⁴N nucleus → three-line pattern



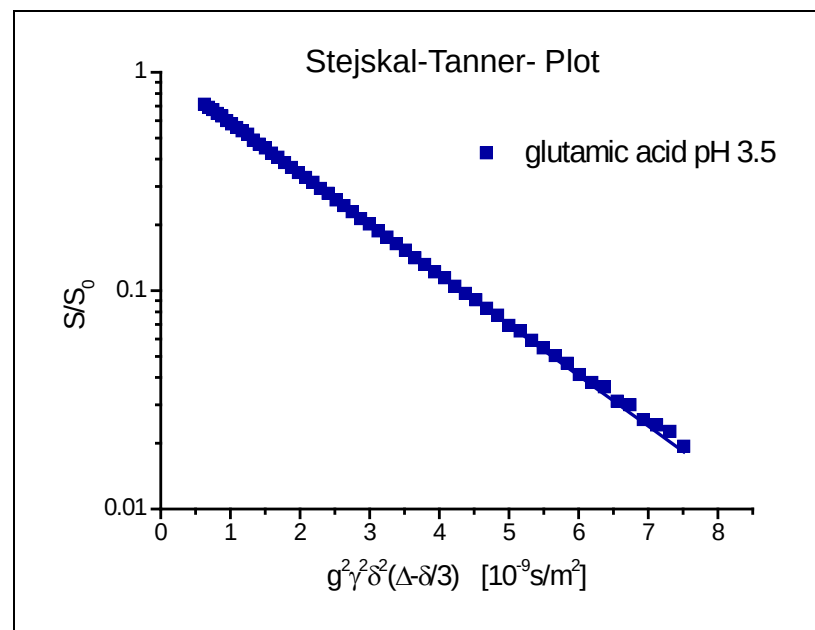
- Poly(diallyldimethylammonium chloride (PDADMAC) and TEMPO-labeled poly(ethylene-alt-maleic acid) (TEMPO-P(E-alt-MA))



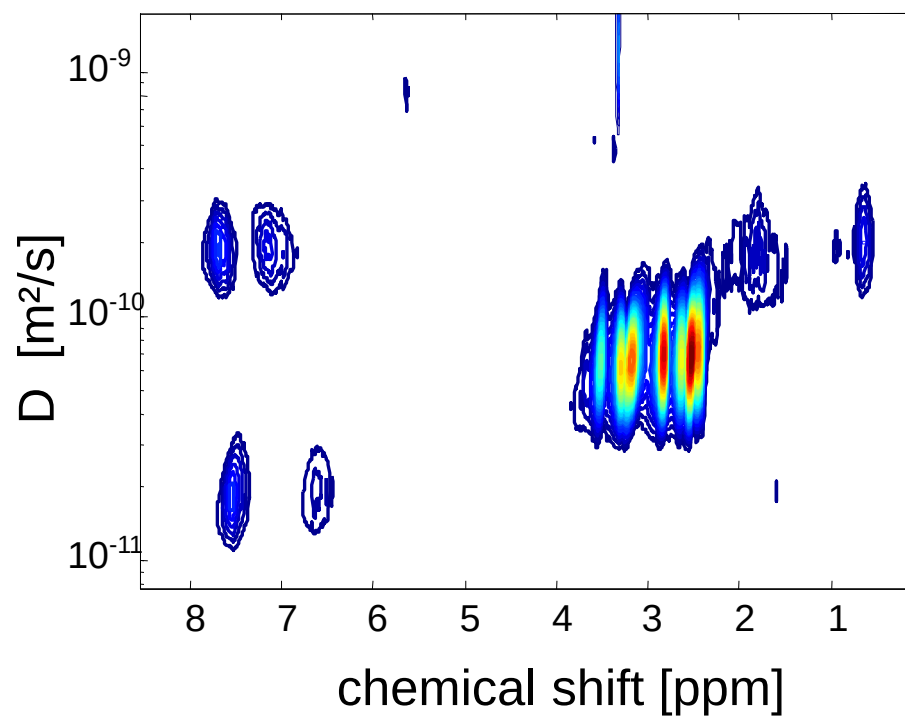
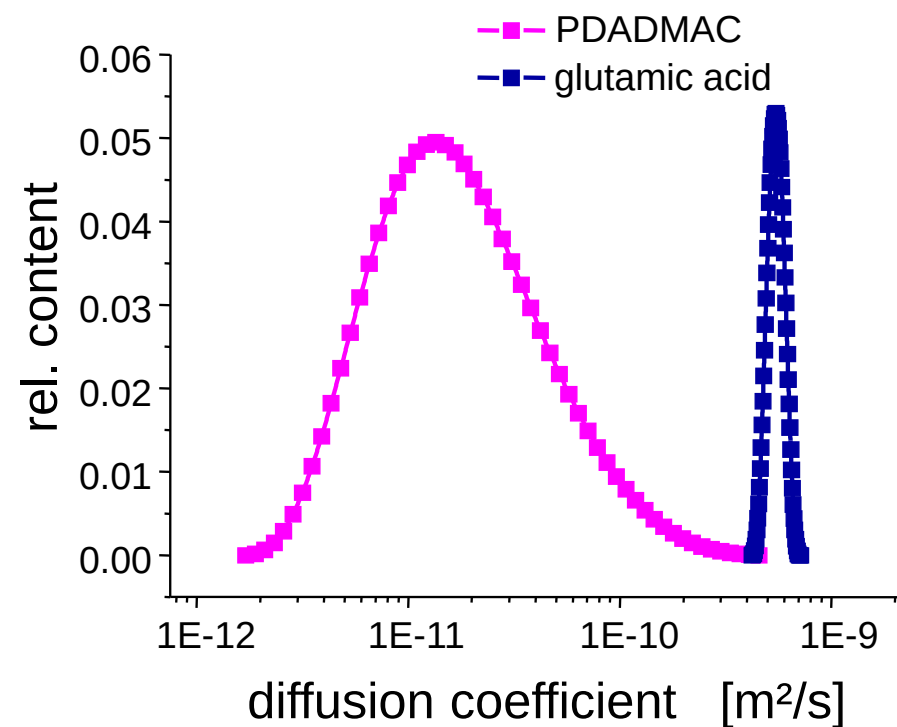
PDADMAC, glutamic acid, water



$$S(g) = S_0 \exp \left[-D \gamma^2 \delta^2 g^2 \left(\Delta - \frac{\delta}{3} \right) \right]$$

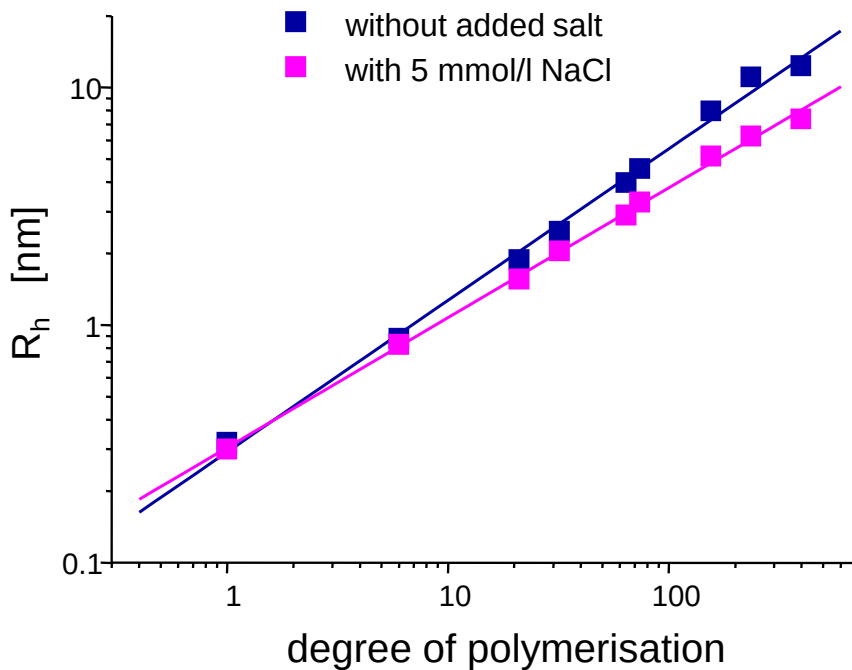


multi-component fit
Contin, cummulant analysis
Inverse Laplace Transform (DOSY)



Stokes- Einstein equation

$$D_o = \frac{k_B T}{f} = \frac{k_B T}{6\pi\eta R_h}$$



Fractal dimension:

PSS

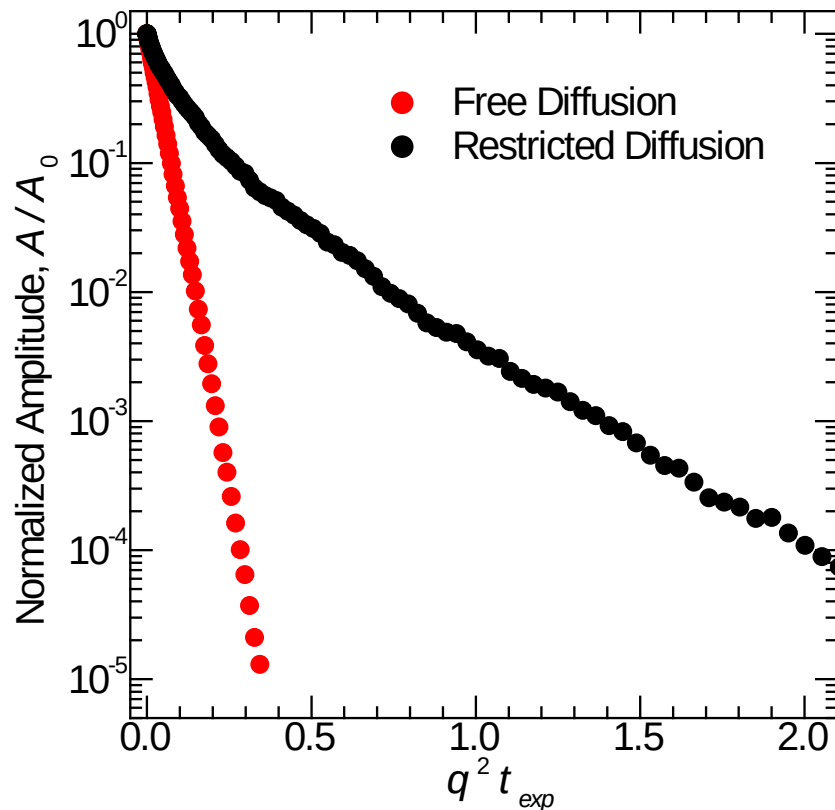
1.6

PSS with 5mmol/l NaCl

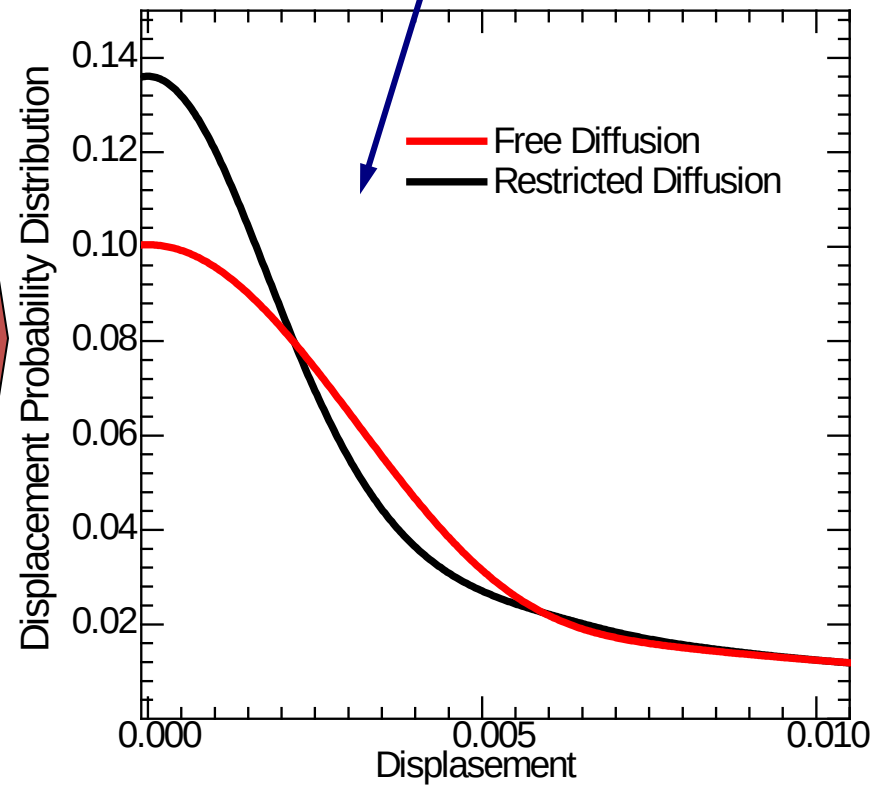
1.8

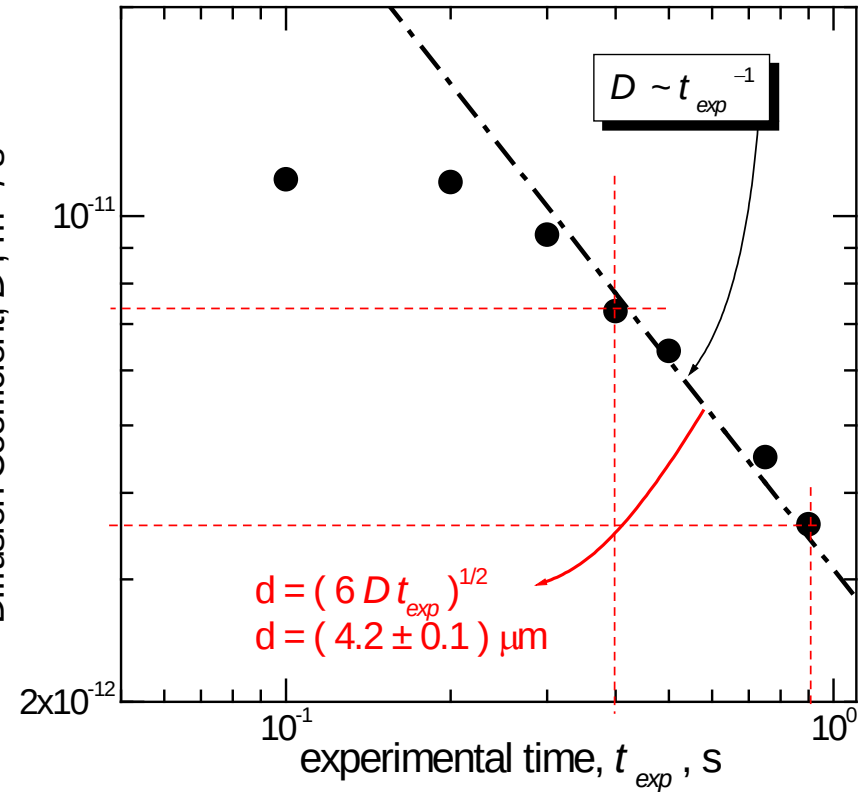
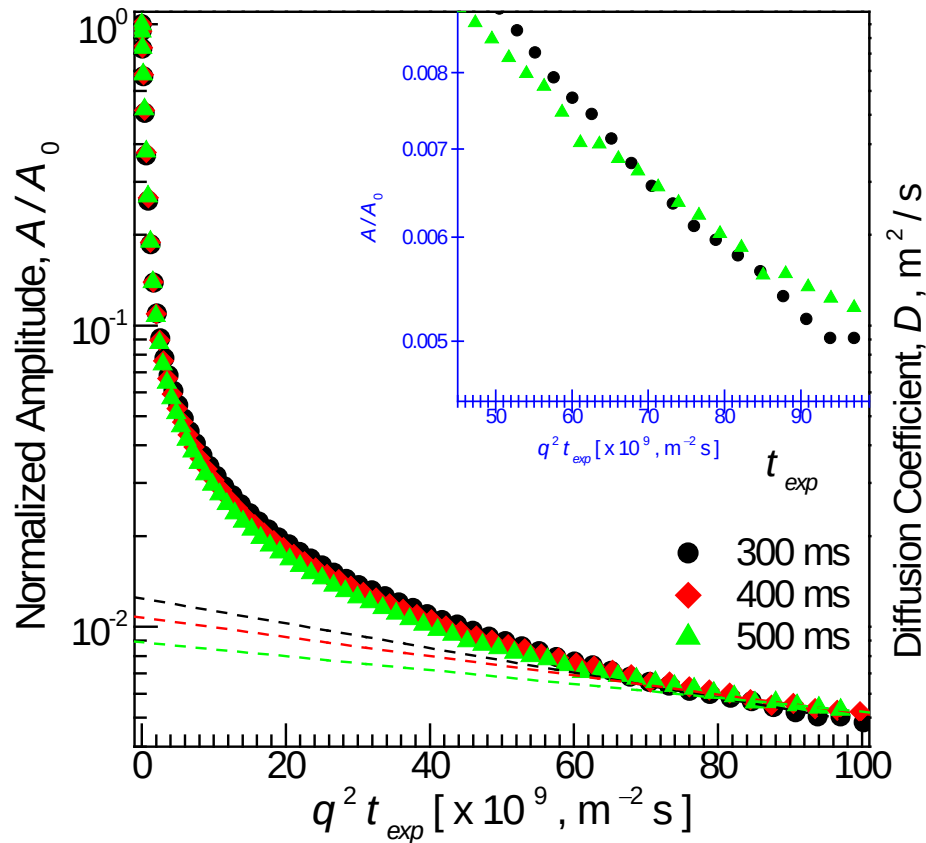
$$A(q, t_{\text{exp}}) = \int \overline{P(r_{m.s.d}, t_{\text{exp}})} \exp(-i2\pi q r_{m.s.d}) dr_{m.s.d}$$

$$A(q, t_{\text{exp}}) \rightarrow \text{inverse-FT} \rightarrow \overline{P(r_{m.s.d}, t_{\text{exp}})} \quad \text{PROPAGATOR}$$



FFT





- flow pattern
- mixing and phase separation
- local mobility responding to external shear
- local mobility site-specific
- hydrodynamic size / micro viscosity
- restricted diffusion