The Neutron Spin Echo Spectrometer at the NIST Center for Neutron Research (NCNR)

Antonio Faraone

Outline

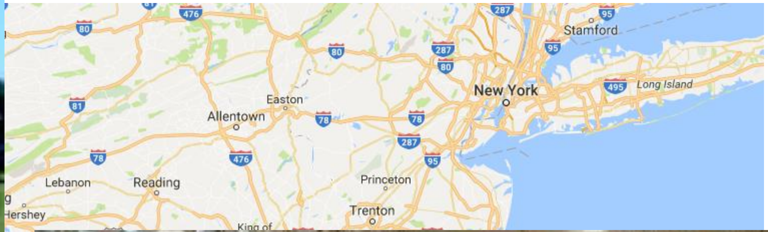
- The NIST Center for Neutron Research (NCNR)
- NSE at NCNR (characteristics)
- Examples of Science carried out with NSE
- Combined use with other instruments (nuclear scattering)

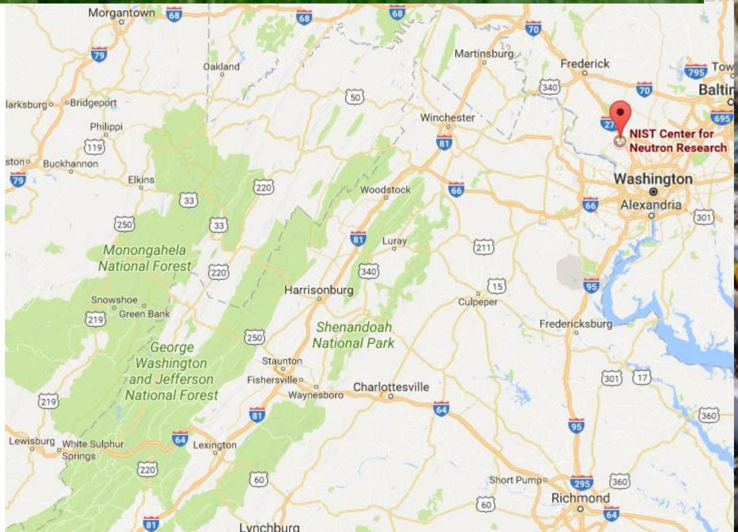
  - Normalization

  - Coherent and incoherent contributions

NIST Center for Neutron Research

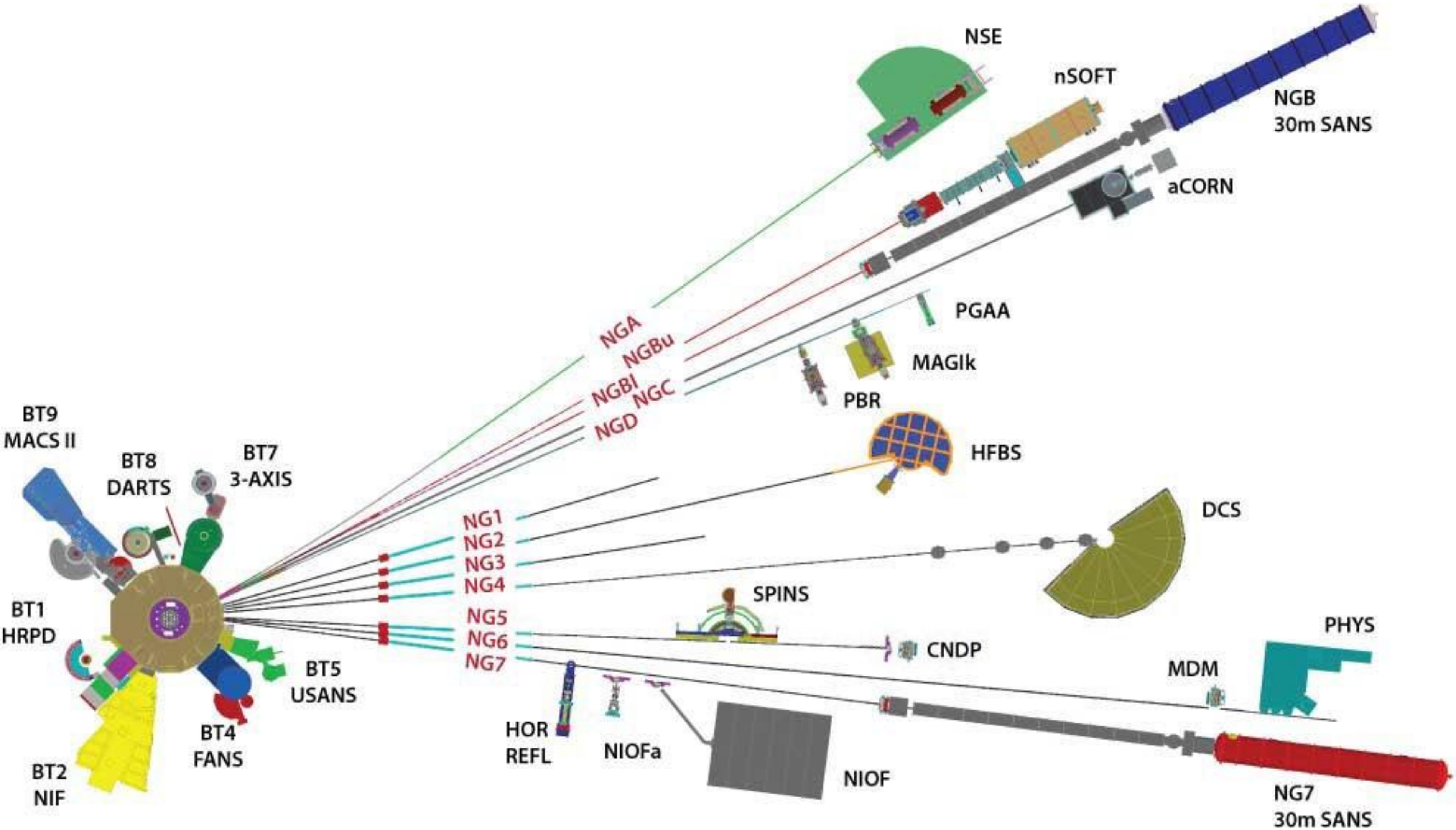
Location: Gaithersburg, MD
Power Source: NBSR 20 MW split core reactor
Operation cycle: ≈7 cycles of 38 days/year (≈260 days/year)
Main Funding: DoC; NSF



NIST Center for Neutron Research

The NSE was moved from its original location on NG-5 to its current position on NG-A in 2014.



NSE at the NCNR

NSE at the NCNR

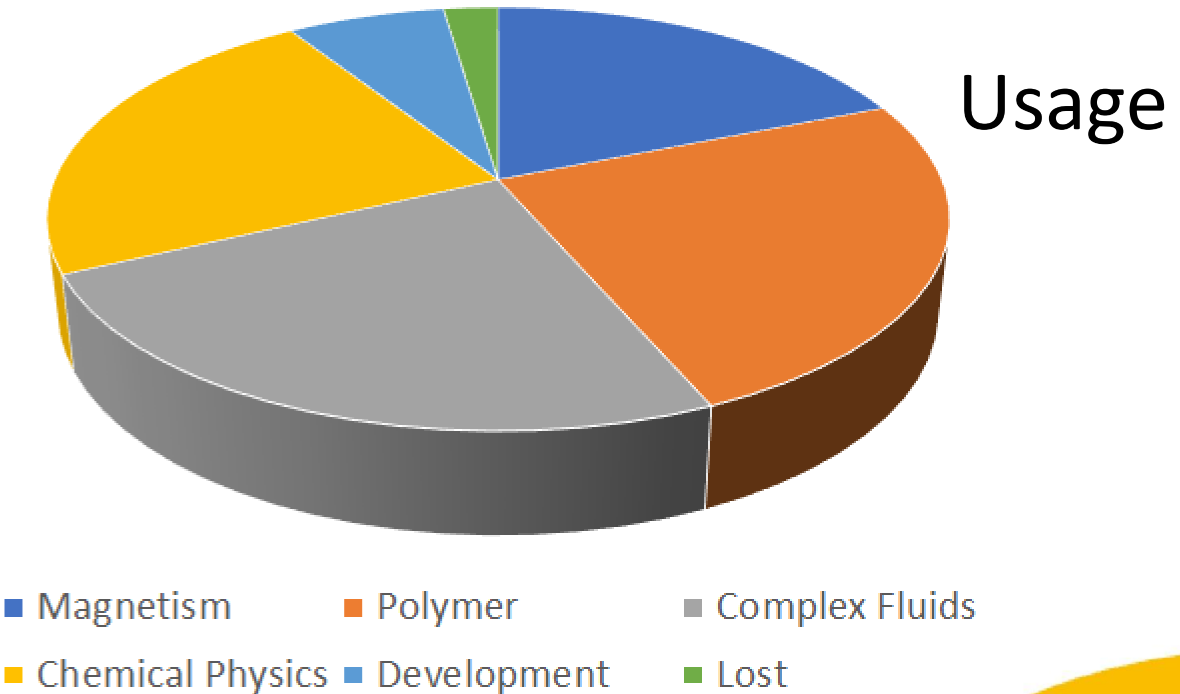
Replica of the NSE at Juelich and later at FRM-II

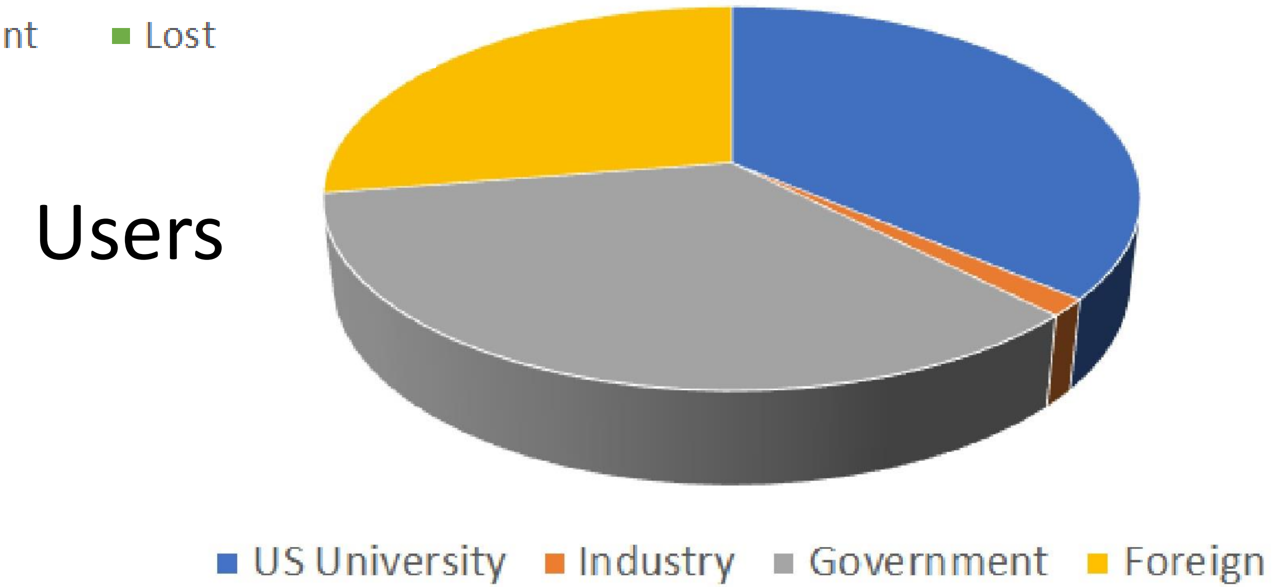
In its new location:

- New PSs
- Same Flux
- New double V transmission polarizer
  - FR ≈30-40 in the whole λ range of use
  - For certain experiments measurement rate x7

Guide	NG-A, 50 mm x 70 mm
λ	4.5 Å to 17 Å
Maximum field integral	≈0.44 T·m
Typical sample size	3 cm x 3 cm
Accessible scattering angle	from 2° to 105°
Accessible Q	from ≈0.06 $Å^{-1}$ to ≈1.8 Å-1 at λ=5 Å
	from ≈0.035 $Å^{-1}$ to ≈1.1 Å-1 at λ=8 Å
	from ≈0.025 $Å^{-1}$ to ≈0.8 Å-1 at λ=11 Å
Dynamic range	from 3 ps to 10 ns at λ=5 Å
	from 10 ps to 40 ns at λ=8 Å
	from 50 ps to 100 ns at λ=11 Å
Detector	32 cm x 32 cm PSD

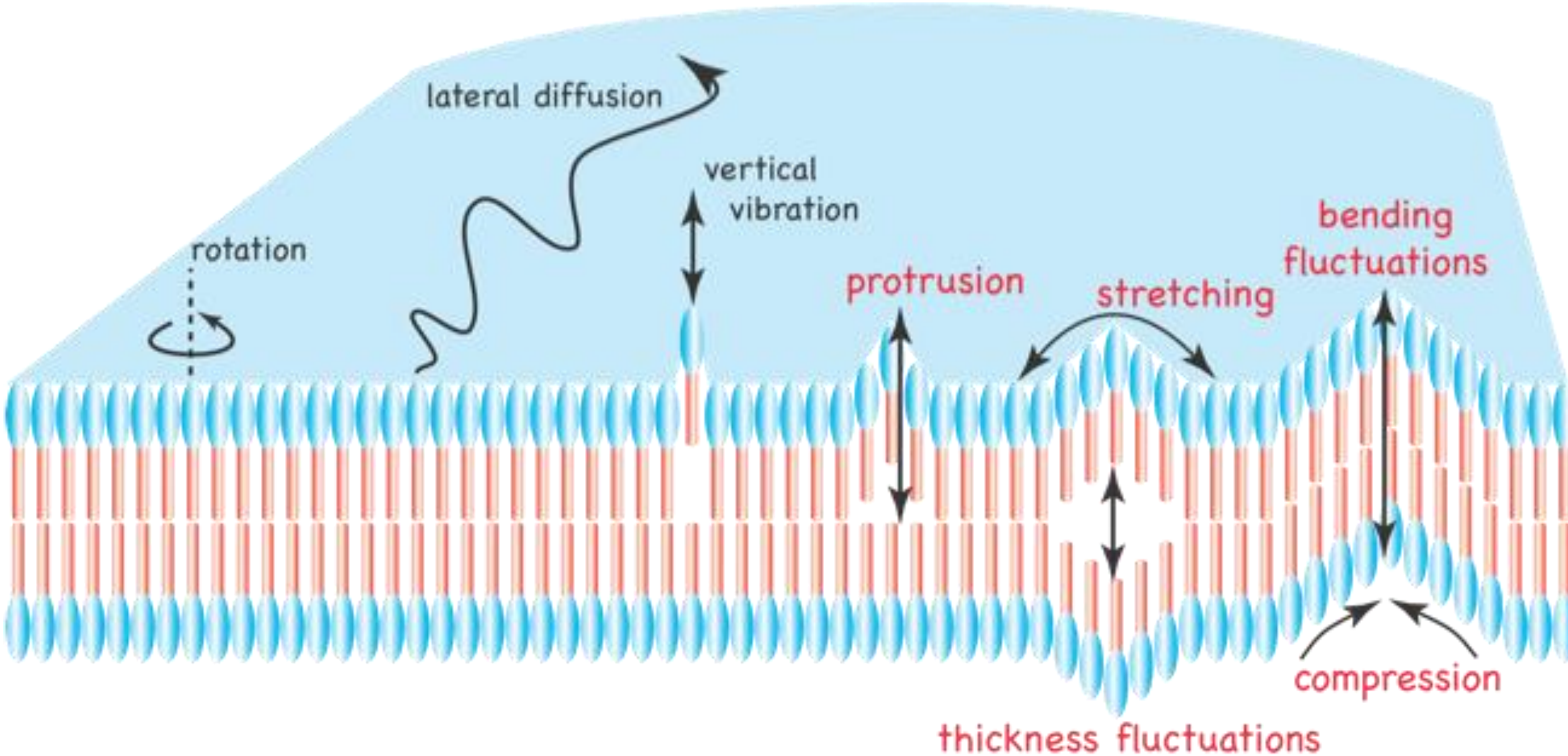
NCNR-NSE: Usage and Users





Phospholipid Membranes Dynamics

observation length scale



molecular motion

collective motion

incoherent-quasi-elastic scattering
nuclear magnetic resonance
etc.

coherent-quasi-elastic scattering
photon correlation spectroscopy

Thickness Fluctuations

- Fluid Phase: Enhancement of the dynamics at Q values corresponding to the bilayer thickness = Thickness Fluctuations
- Gel Phase: Bending Dynamics only.

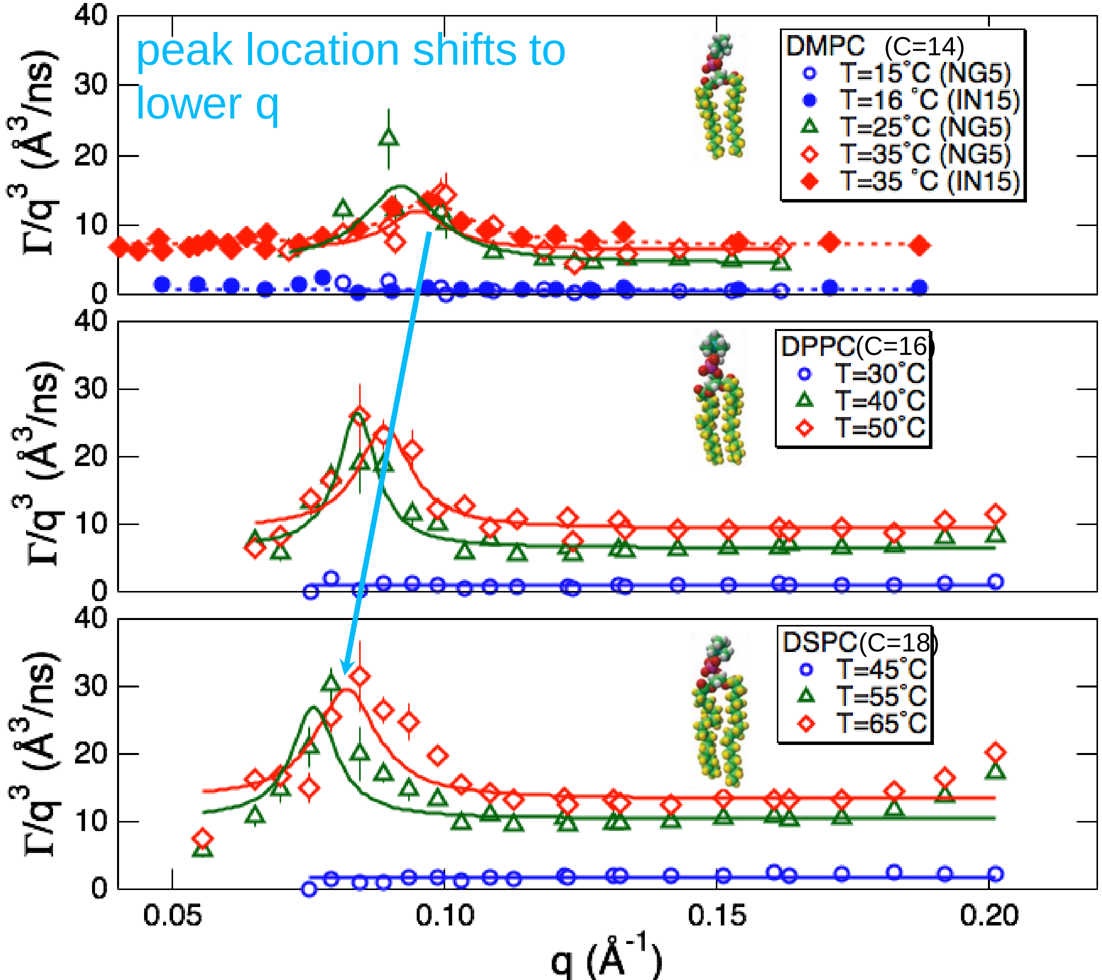
Empirical Fit Equation

$$\frac{\Gamma}{q^3} = \frac{\Gamma_{BD}}{q^3} + \frac{(\tau_{TF} q_0^3)^{-1}}{1 + (q - q_0)^2 \xi^2}$$

Γ_{BD} Bending Modulus

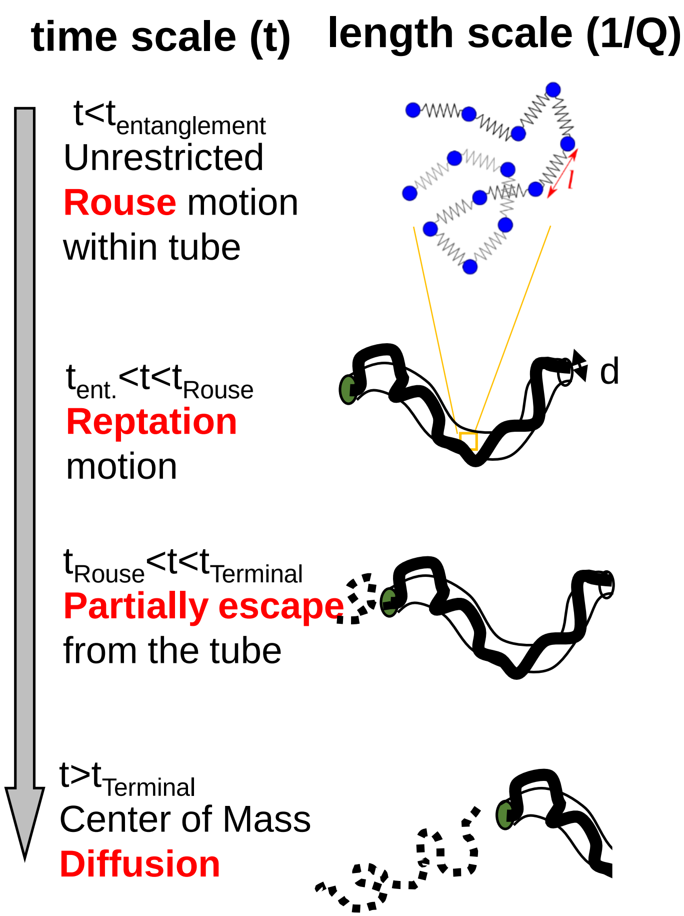
τ_{TF} Relaxation Times

$d_m/\xi q_0$ Fluctutation Amplitude

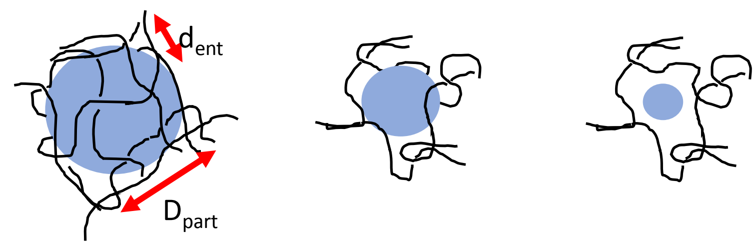


Woodka et al., *PRL*, **109**, 058102 (2012)

Polymer Dynamics in Nanocomposites

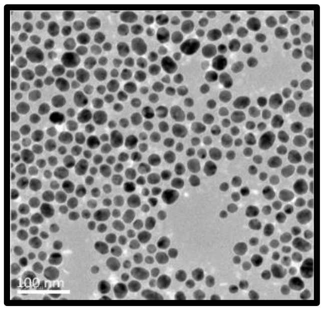


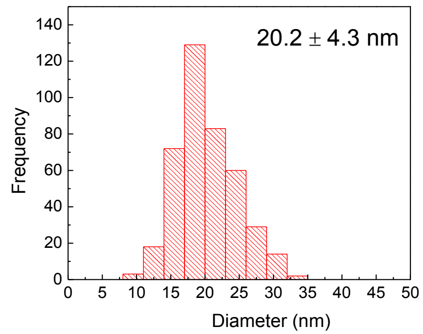
The power of small



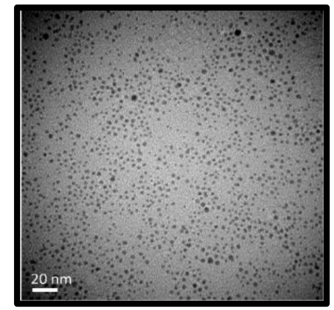
Gold Nanoparticles Composites

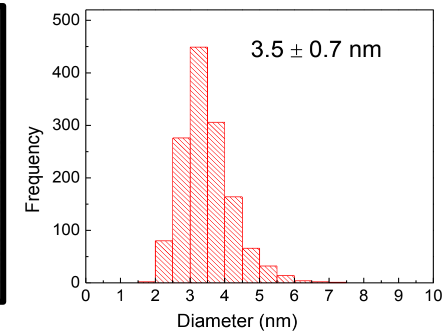
Large NPs





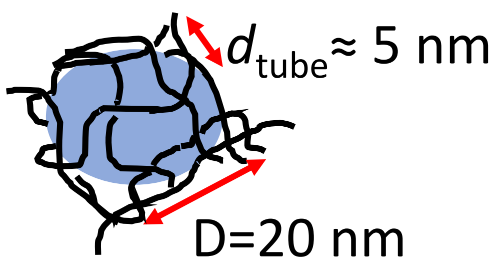
Small NPs

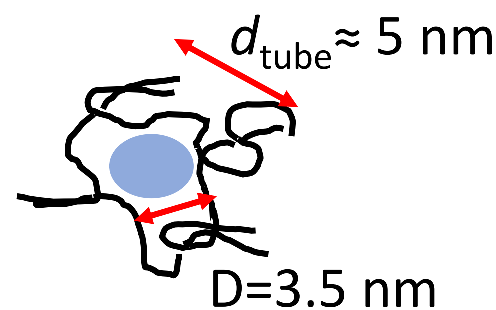




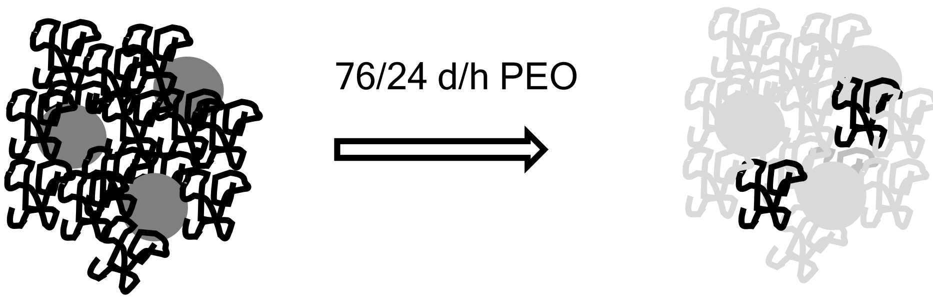
Particles are PEG coated (< 1nm) to provide entropic stabilization

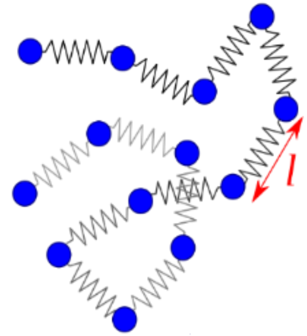
We made nanocomposites with these particles (20 % by volume) and long chain poly (ethylene glycol) (PEG) matrix (35 kg/mol).

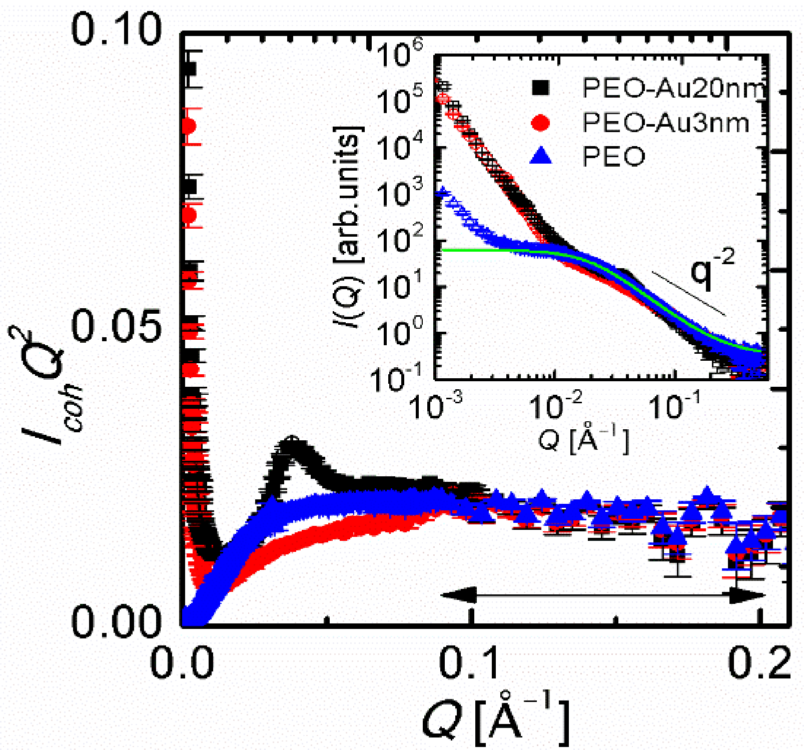


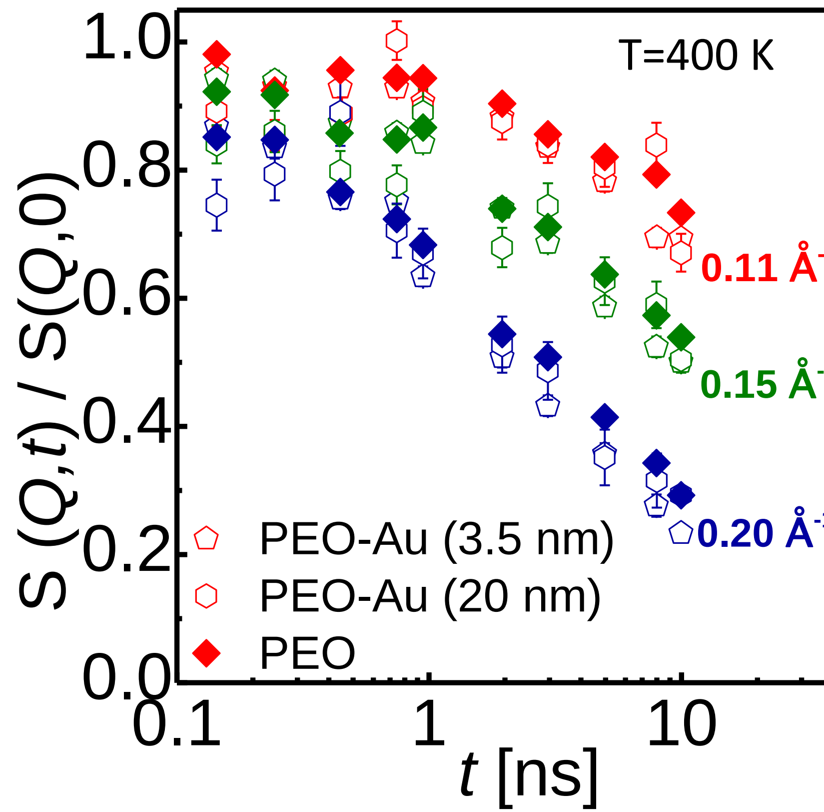


Short time behavior - *Rouse dynamics*





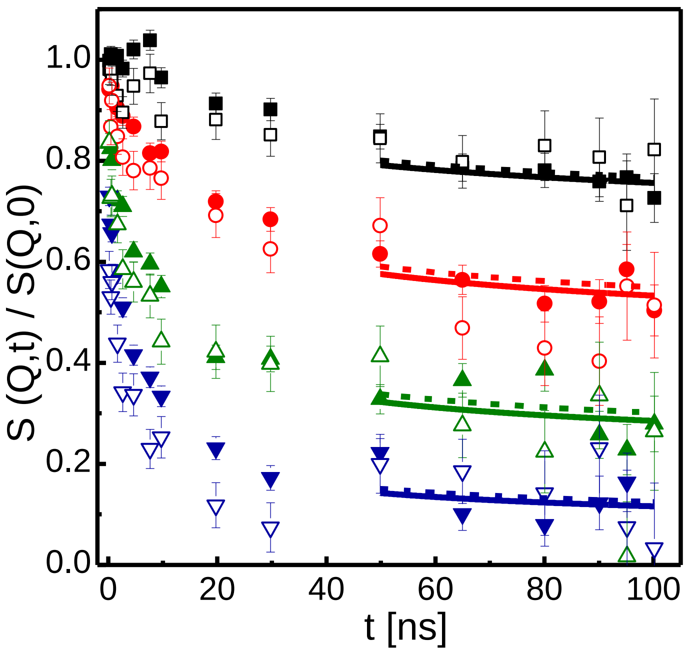




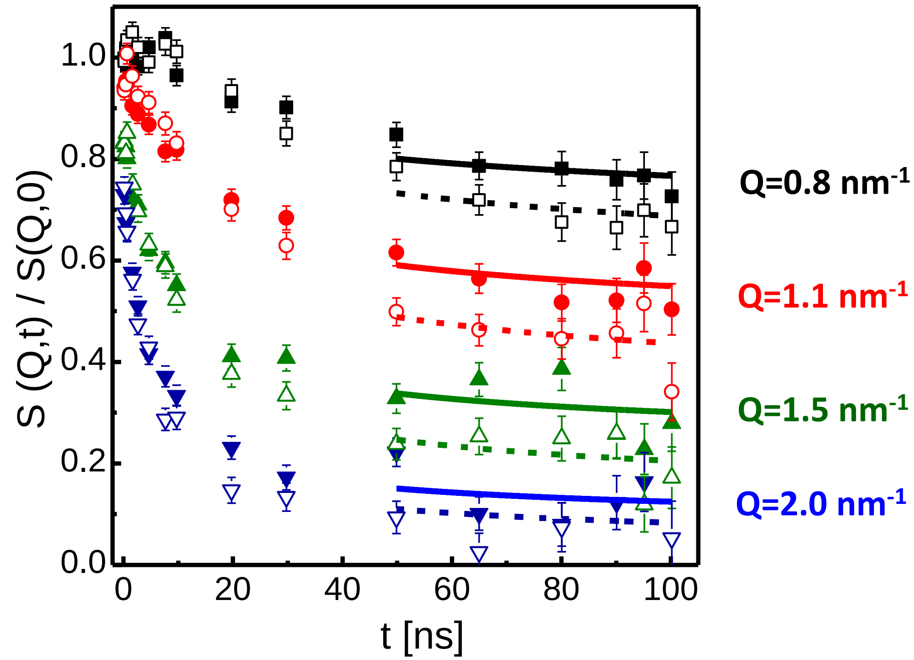
Rouse dynamics is not modified

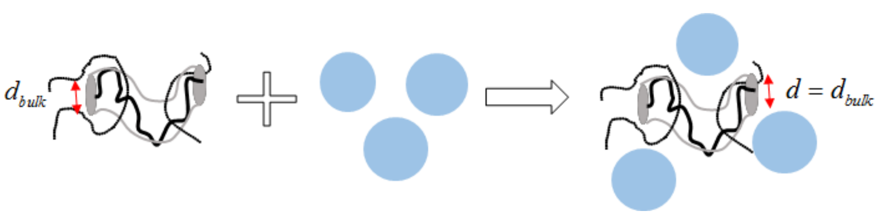
Long time behavior - *Confined motion*

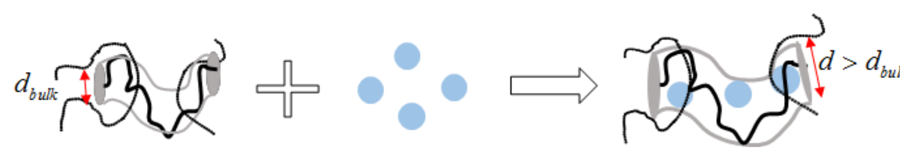
PNC with 20 nm particles



PNC with 3.5 nm particles







$$d_{PEO} = 5.03 \pm 0.1 \text{ nm}$$
$$\approx$$
$$d_{PEO-20nmAu} = 5.17 \pm 0.19 \text{ nm}$$

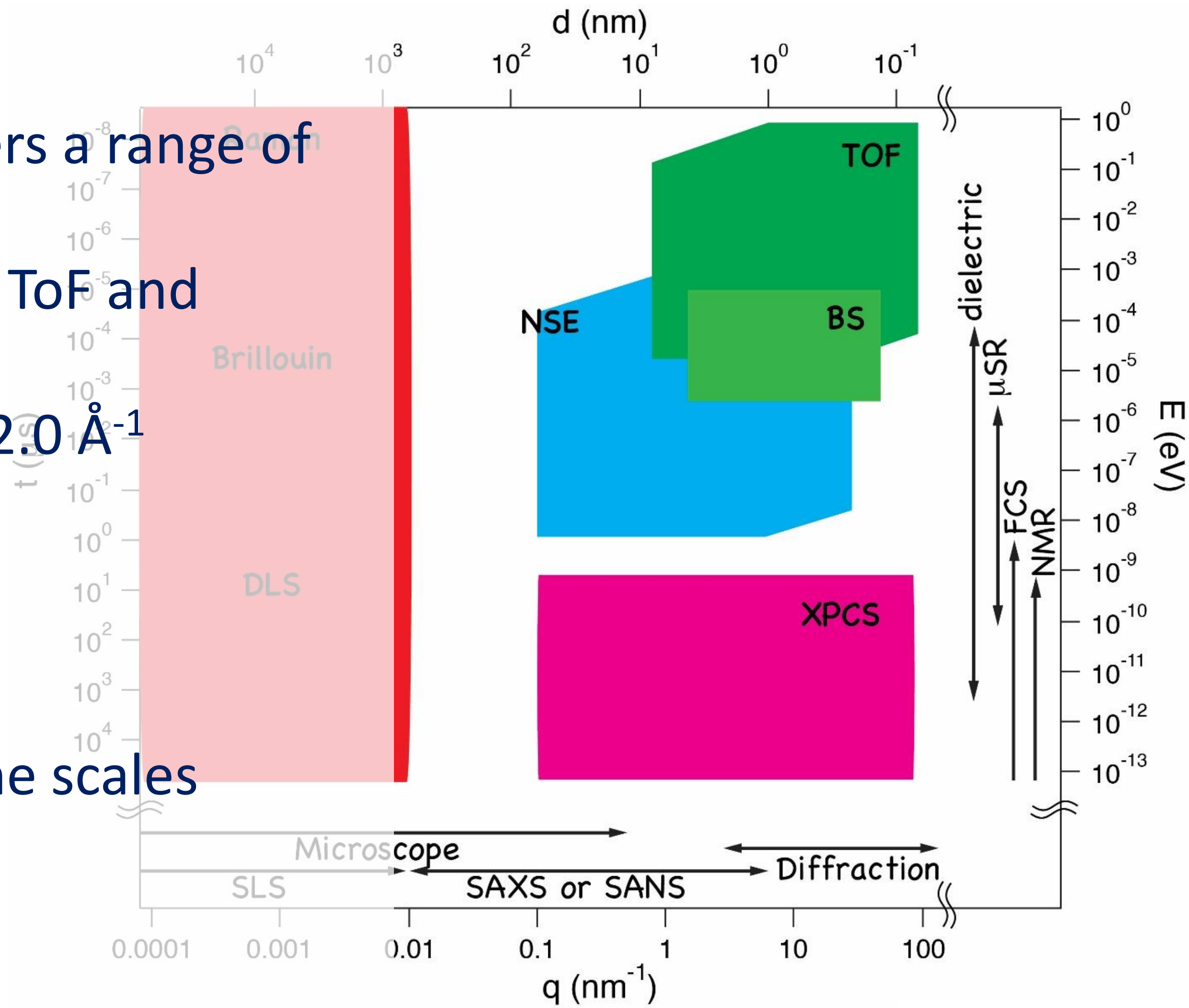
$$d_{PEO} = 5.03 \pm 0.1 \text{ nm}$$
$$<$$
$$d_{PEO-3nmAu} = 6.11 \pm 0.13 \text{ nm}$$

Senses et al., *PRL*, **118**, 147801 (2017)

Getting Together Data from Different QENS Instruments

- When?
  - NSE uniquely covers a range of low Q (< ≈0.3 Å-1)
  - NSE overlaps with ToF and Backscattering for

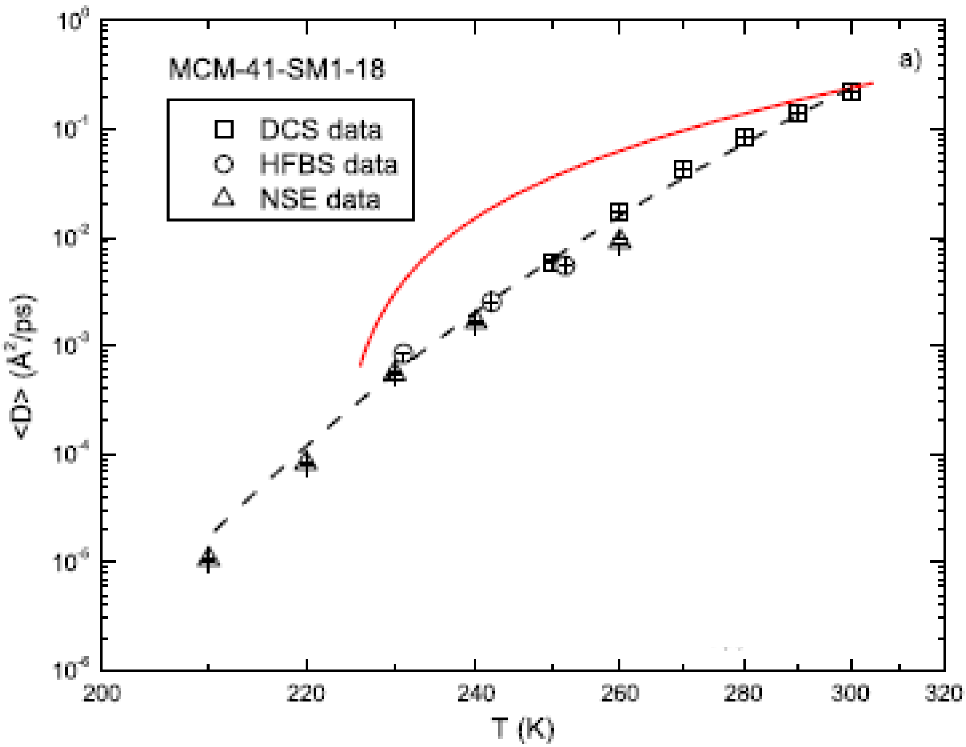
    $\approx 0.3\ Å^{-1} < Q < \approx 2.0\ Å^{-1}$
  - Chemical Physics
- Why?
  - Validate results
  - Access shorter time scales



Courtesy of MN

Easiest case different temperatures

Water Dynamics in a Nanoporous matrix



- Independent analysis
- Satisfactory model
- Information contained in the spectra of each instruments separately

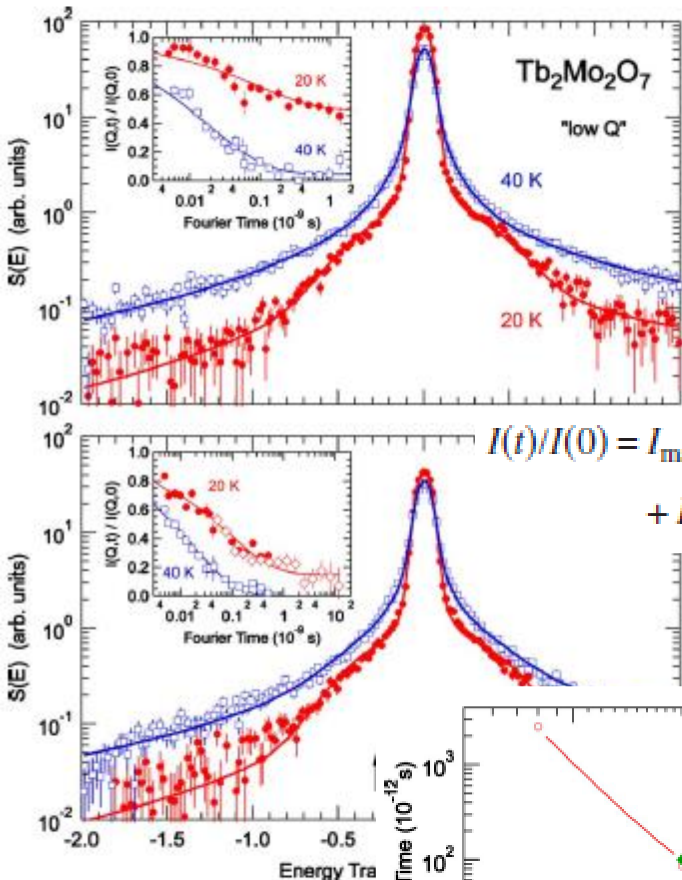
THE JOURNAL OF CHEMICAL PHYSICS **130**, 134512 (2009)

Single particle dynamics of water confined in a hydrophobically modified MCM-41-S nanoporous matrix

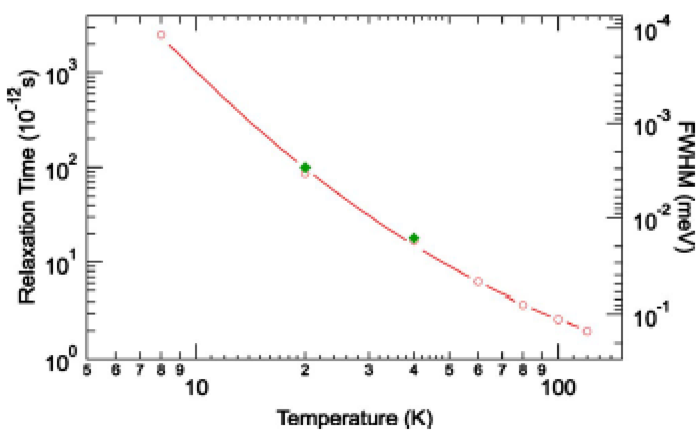
Antonio Faraone,[1,a] Kao-Hsiang Liu,[2] Chung-Yuan Mou,[2] Yang Zhang,[3] and Sow-Hsin Chen[3]

Most Rigorous approach

Global fitting of different data



$$I(t)/I(0) = I_{mag}/I(0) + I_{CF}/I(0) \cdot \mathcal{F}^{-1}\{g(\pm\hbar\omega_0)\} + I_{QE}/I(0)\exp(-[t/\tau]^{\beta}),$$



- Not straightforward to implement
- For expert users
- Requires previous knowledge of appropriate model

PHYSICAL REVIEW B **81**, 224405 (2010)

High-resolution neutron scattering study of $Tb_2Mo_2O_7$: A geometrically frustrated spin glass

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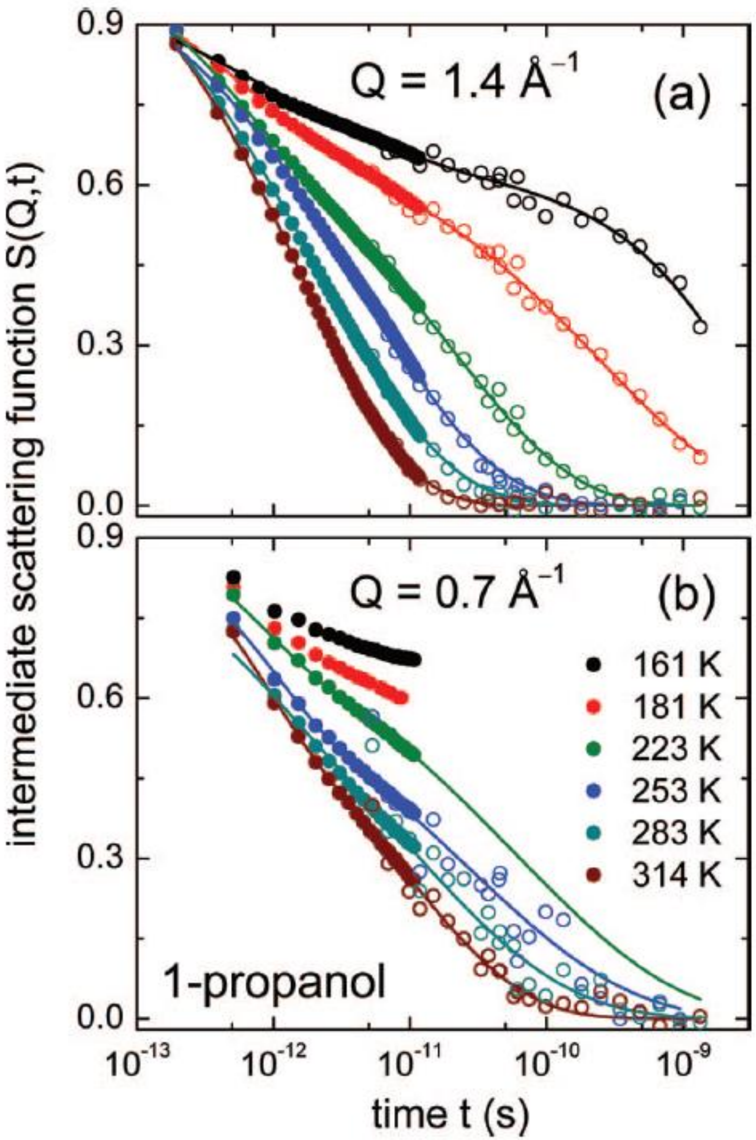
(Received 31 March 2010; revised manuscript received 3 May 2010; published 2 June 2010)

Overlap of data

Dynamics of liquid (propanol)



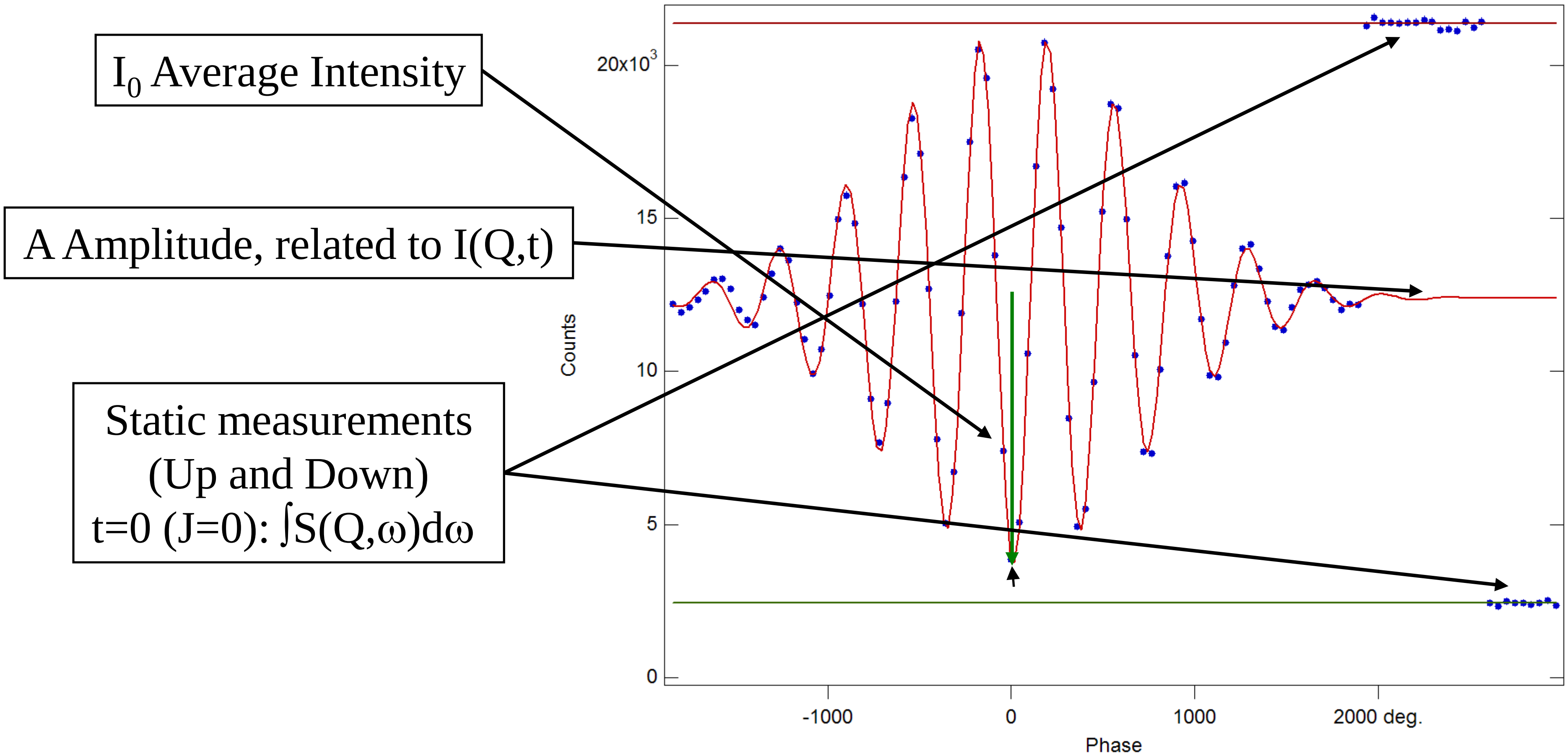
- Requires Fourier Transform of experimental data

THE JOURNAL OF CHEMICAL PHYSICS **140**, 124501 (2014)

Liquid 1-propanol studied by neutron scattering, near-infrared, and dielectric spectroscopy

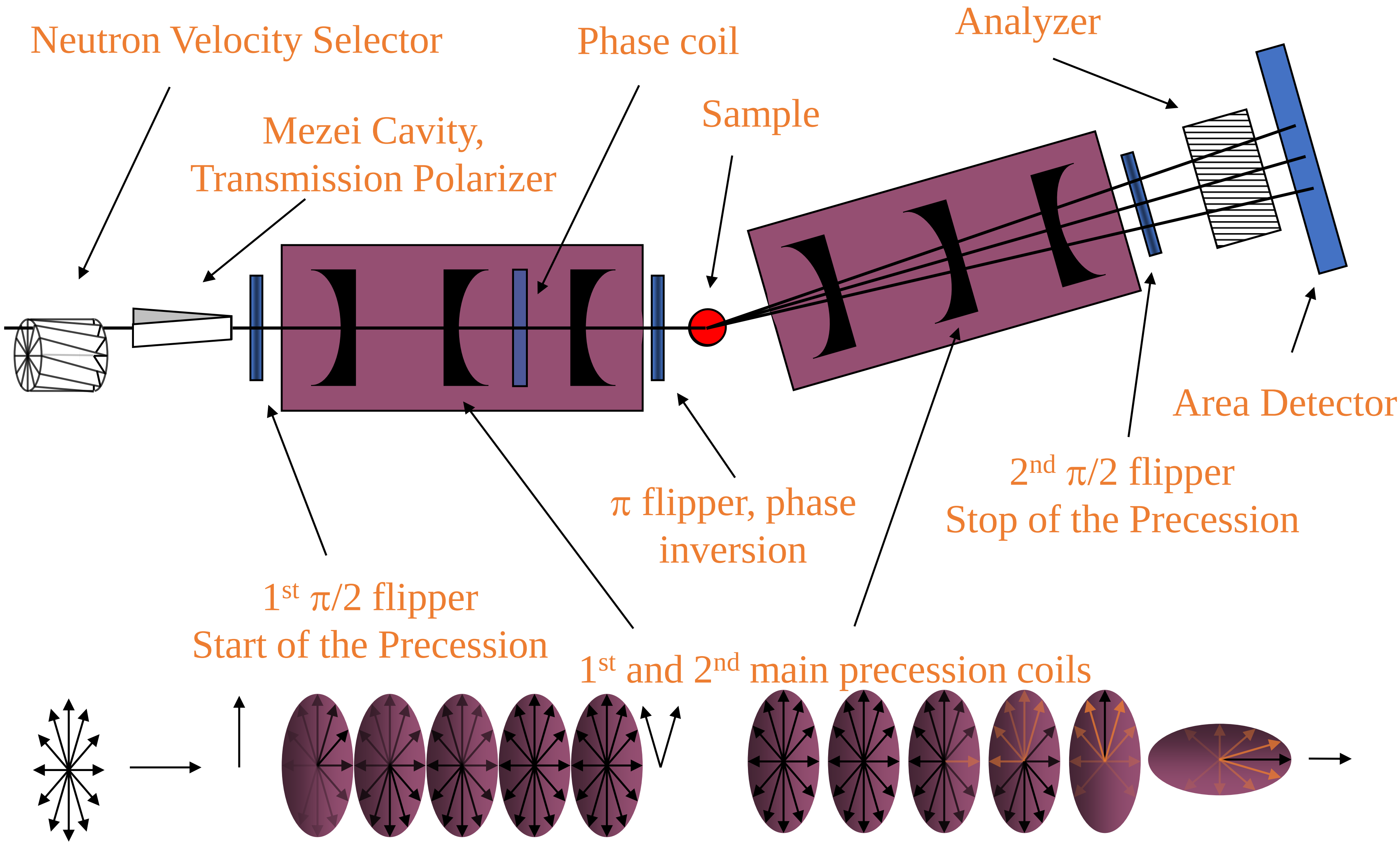
P. Sillrén,[1] A. Matic,[1] M. Karlsson,[1] M. Koza,[2] M. Maccarini,[2] P. Fouquet,[2] M. Götz,[3] Th. Bauer,[3] R. Gulich,[3] P. Lunkenheimer,[3] A. Loidl,[3] J. Mattsson,[4] C. Gainaru,[5] E. Vynokur,[5] S. Schildmann,[5] S. Bauer,[5] and R. Böhmer[5]

How we measure…



$$\frac{I(Q,t)}{I(Q)} = \frac{2A}{Up - Dwn}$$

Polarization Analysis (Nuclear Scattering)



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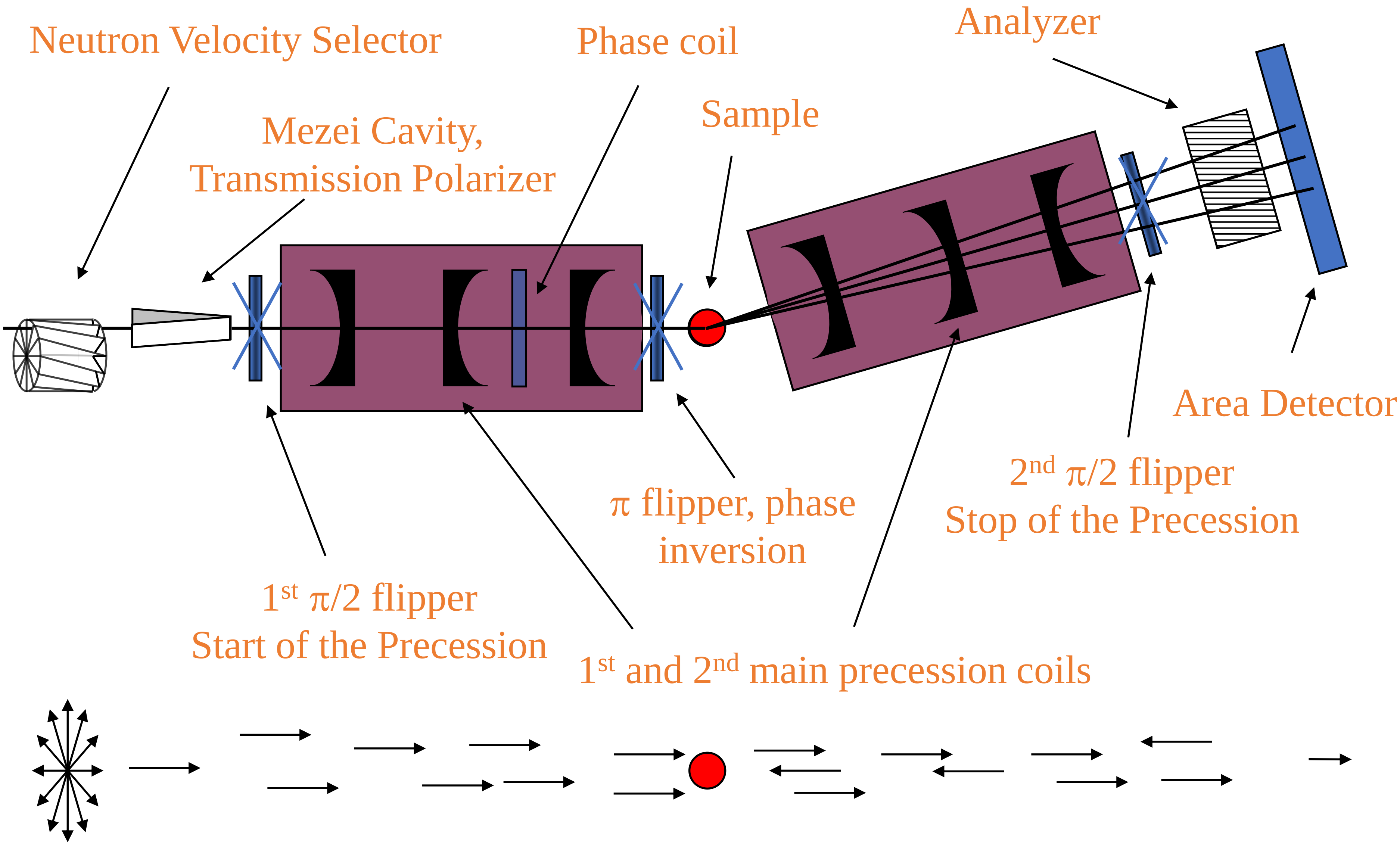
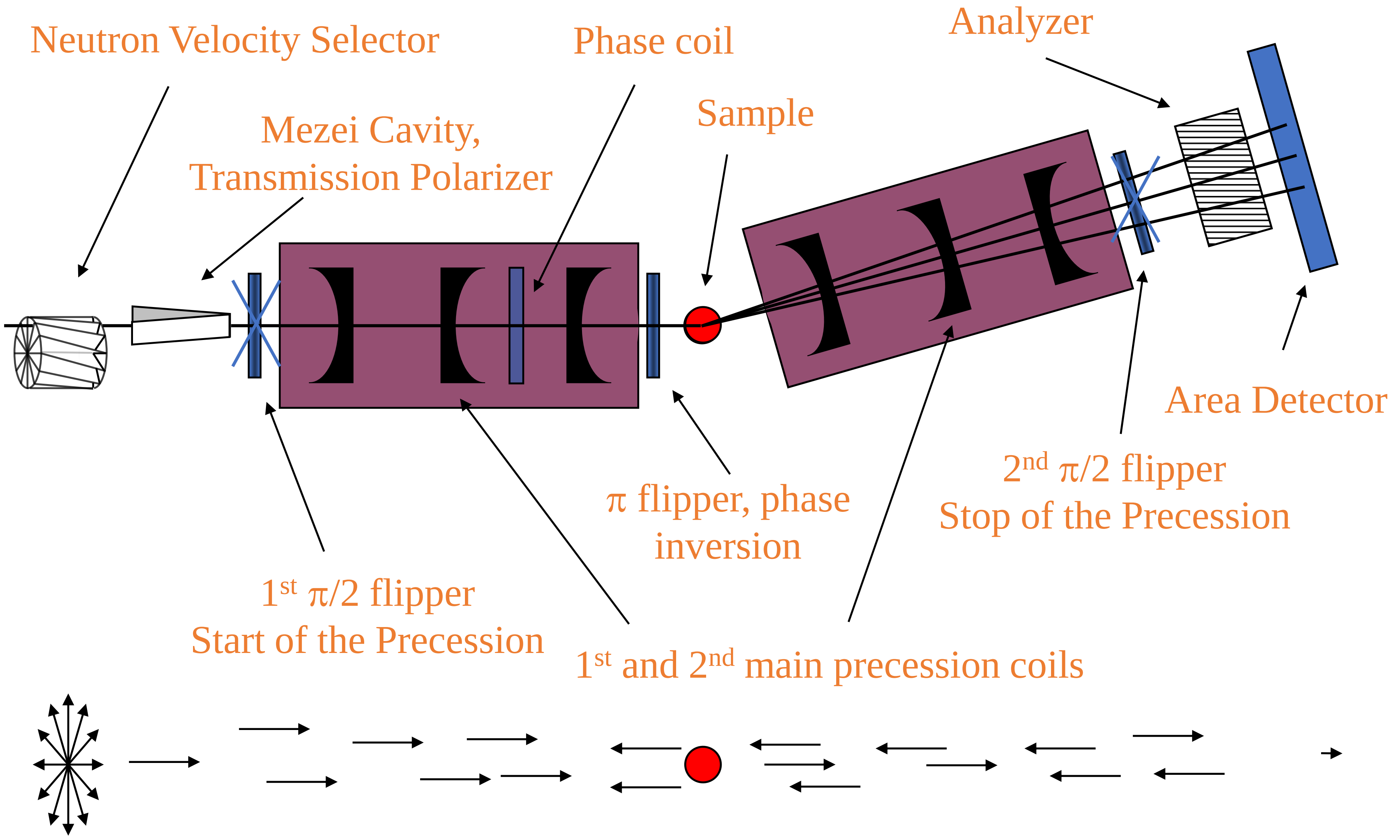


Polarization Analysis (Nuclear Scattering)



What it is measured

$$S^{QENS}(Q,E) = S^{coh}(Q,E) + S^{inc}(Q,E)$$

$$\frac{I^{NSE}(Q,t)}{I^{NSE}(Q)} = \frac{I^{coh}(Q,t) - \frac{1}{3}I^{inc}(Q,t)}{I^{coh}(Q) - \frac{1}{3}I^{inc}(Q)}$$

$$I^{coh}(Q,t) = FT\{S^{coh}(Q,E)\} \qquad I^{inc}(Q,t) = FT\{S^{inc}(Q,E)\}$$

$$I^{x}(Q) = I^{x}(Q,t=0) = S^{x}(Q)$$

When coherent or incoherent is dominant

$$I^{NSE}(Q,t) = FT\{S^{QENS}(Q,E)\}$$

The problem of how to normalize the data remain.

The way S(Q) is measured on NSE and on a QENS instrument is different.

- Main issue is fast processes outside the energy window
- Normalizing to base temperature? (DW?)

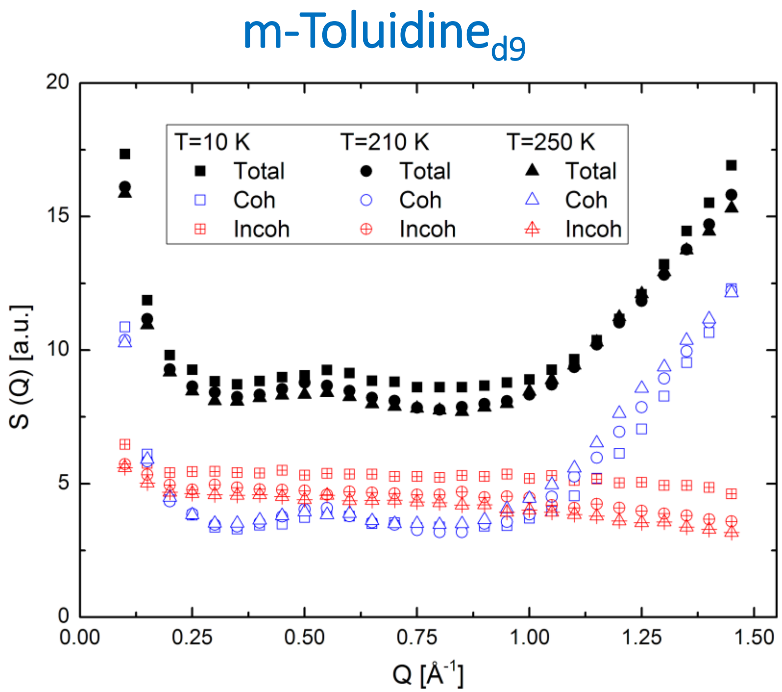
When both contributions are dynamic

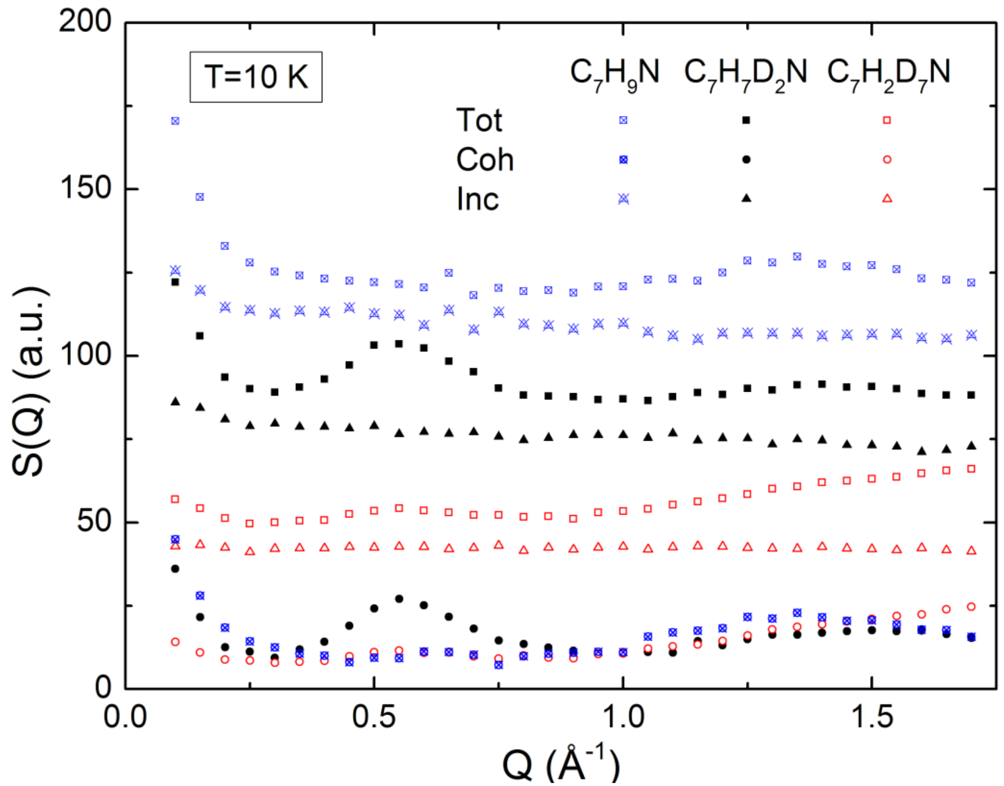
It is an issue common to both QENS and NSE

There is no general way of approaching the problem beyond modeling both contributions

Isotopic substitution might help

Dynamics of a glass former at the prepeak





- Even in the totally deuterated sample, the prepeak coherent intensity is not much higher than the incoherent background.
- The prepeak is stronger in the partially deuterated samples

Combining Spectra (Structure)

$$S_{coh}^{peak}(Q) = F^{C_7H_2D_7N} S_{coh}^{C_7H_2D_7N}(Q) + F^{C_7H_7D_2N} S_{coh}^{C_7H_7D_2N}(Q) - F^{C_7H_9N} S_{coh}^{C_7H_9N}(Q)$$

$$S_{inc}^{peak}(Q) = F^{C_7H_2D_7N} S_{inc}^{C_7H_2D_7N}(Q) + F^{C_7H_7D_2N} S_{inc}^{C_7H_7D_2N}(Q) - F^{C_7H_9N} S_{inc}^{C_7H_9N}(Q) \approx 0$$

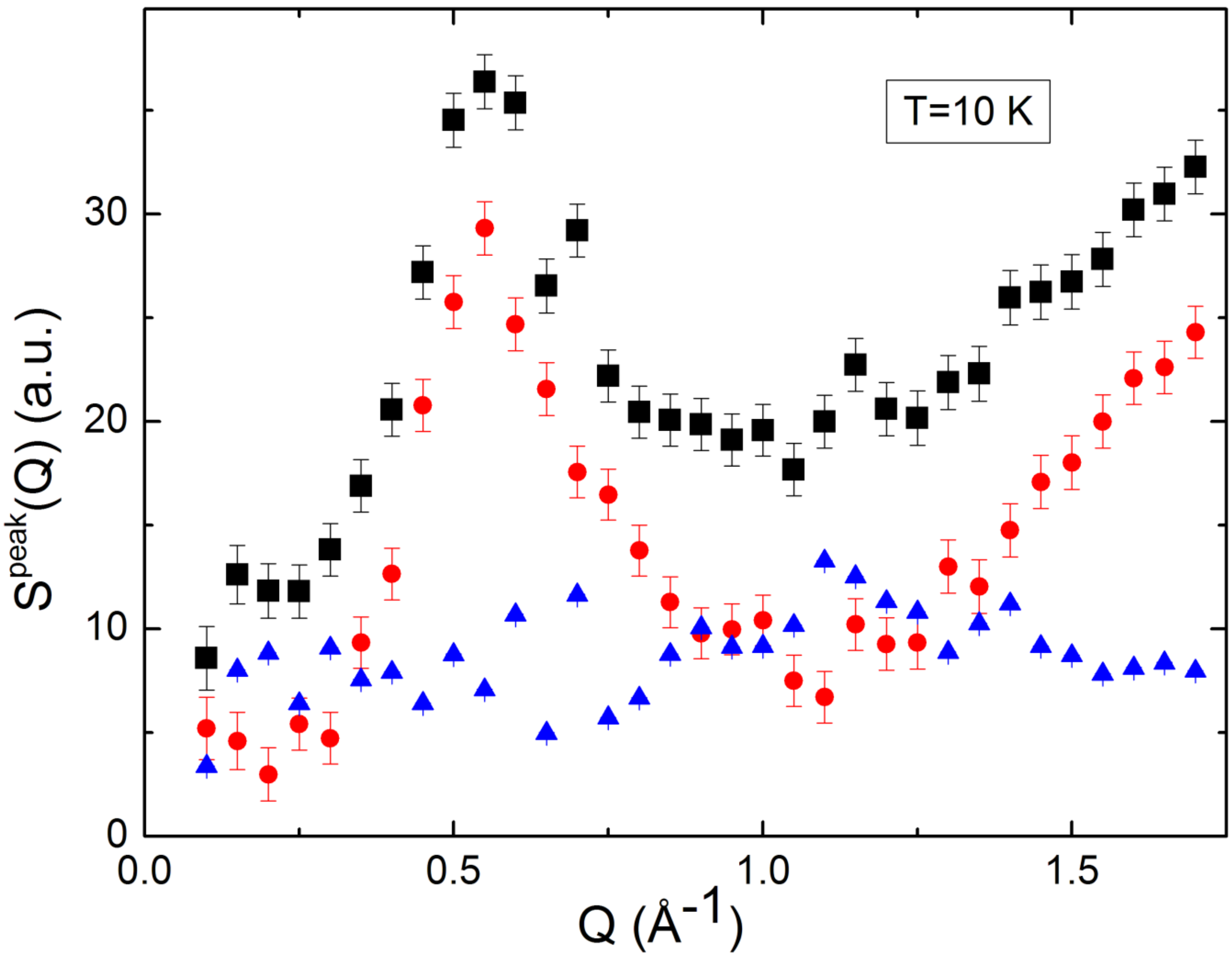
$$F^x = \frac{M_w^x}{M^x T^x};$$

M_w^x molecular weight;

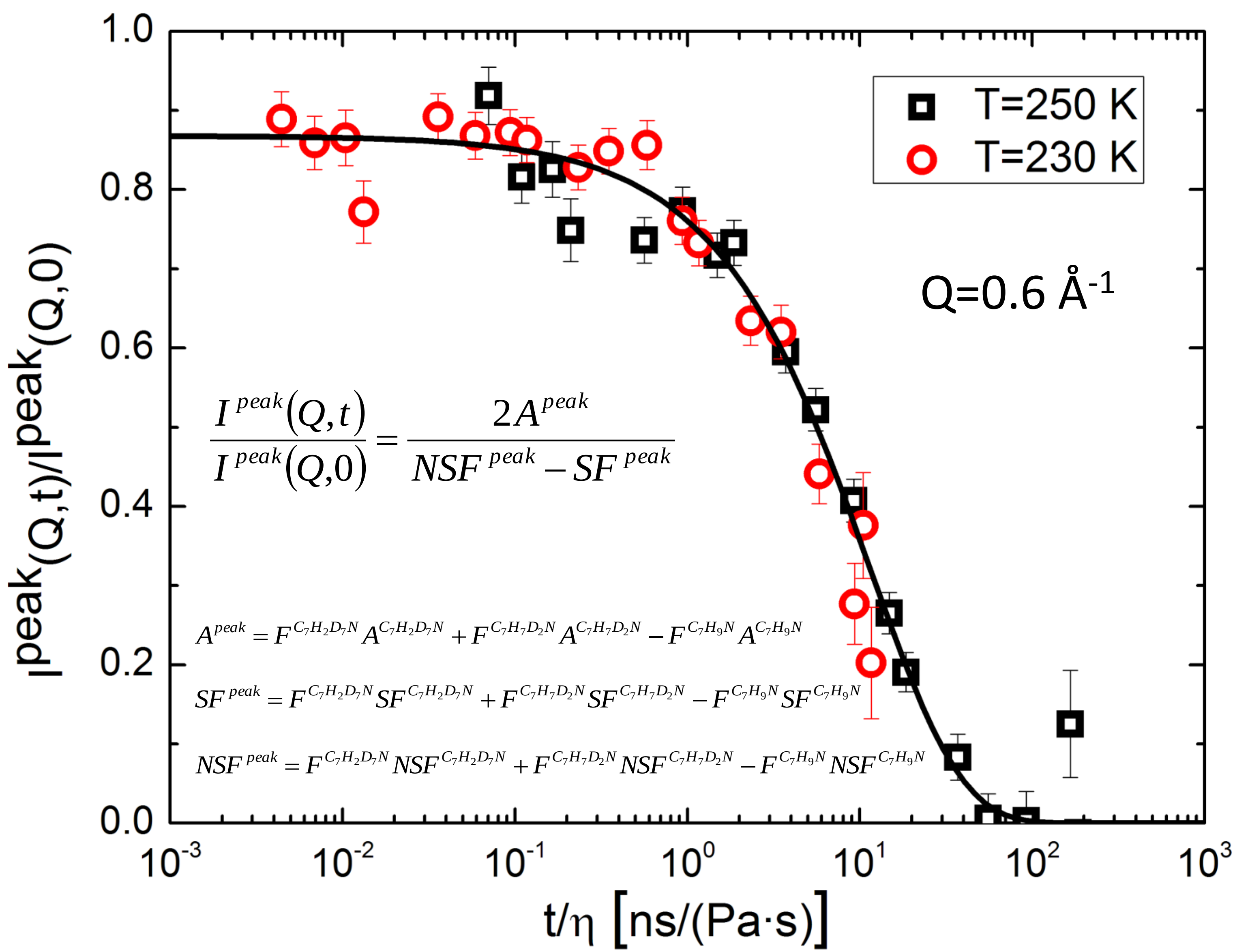
M^x sample Mass;

T^x transmission

$$S^{peak}(Q) = F^{C_7H_2D_7N} S^{C_7H_2D_7N}(Q) + F^{C_7H_7D_2N} S^{C_7H_7D_2N}(Q) - F^{C_7H_9N} S^{C_7H_9N}(Q) \approx S_{coh}^{peak}(Q)$$



Combining Spectra (Dynamics)



Faraone et al., *JCP,* **136**, 104502 (2012)

Take Home Messages

- Do use multiple spectrometer for your investigation (including NSE)
- Be careful to coherent and incoherent relative contributions
- Please, apply for NSE beam time at NCNR

Thank You for Your Attention