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FORSCHUNGSZENTRUM

IKON5 - 26/9/13

High-Resolution Neutron Spin-Echo Spectrometer for ESS

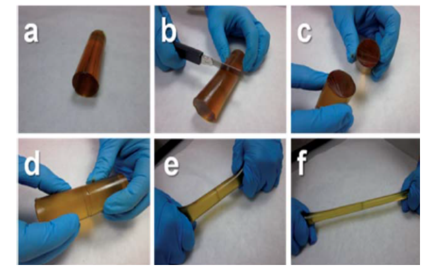
Michael Monkenbusch, Stefano Pasini

NSE-Science Case - dense polymeric systems:

Challenges and new problems:

- <u>new molecular architectures</u>: rings, (semi-)transient double-networks, dendrimers, bottle-brushes, **stars**, combs, blends of those

- <u>new monomers</u>: role of chemical nature



DOI: 10.1039/c3mh00061c

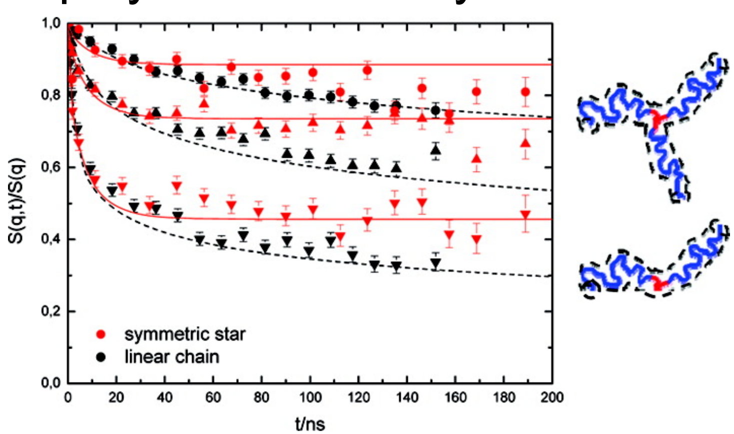
Versus a universal behaviour

- stimulus responsive systems (e.g. photosensitive), **self healing**

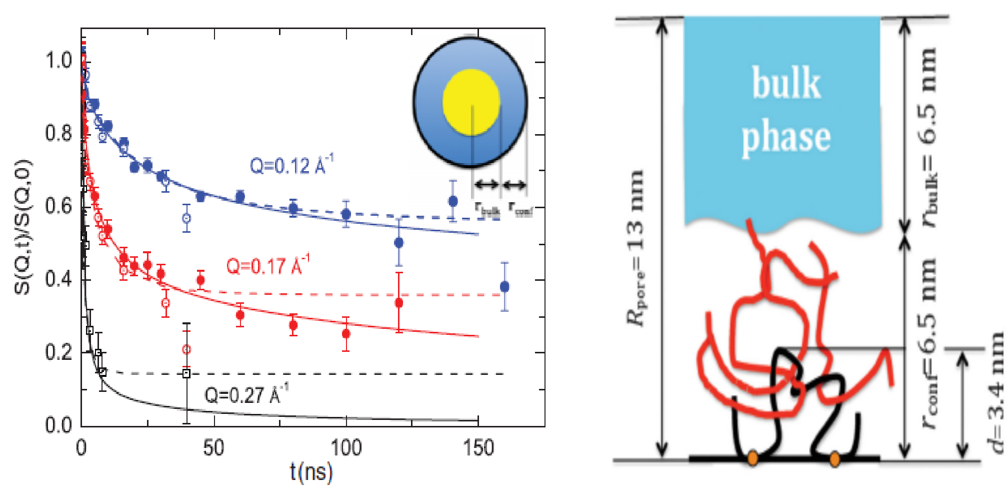
- **confinement in pores**

- interaction with nanoparticles

- polymeric electrolytes



Zamponi et al., *Macromolecules* **2010,** 43, 518-524



Krutyeva et al., PRL 110, 108303 (2013)

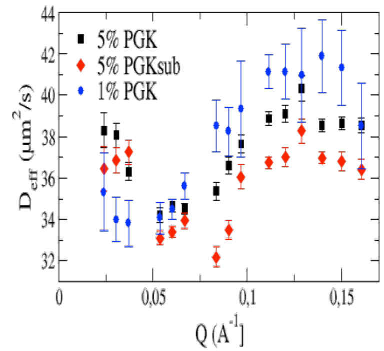
NSE-Science Case – biomolecules:

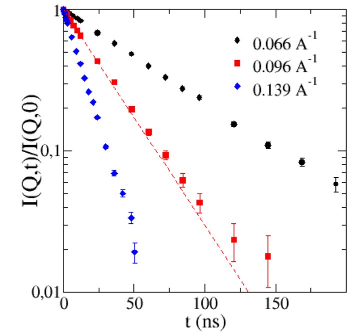
- Functional domain motions in proteins:

mode 7 ! mode 8 mode 9

PGK

approach facilitates chemical reaction

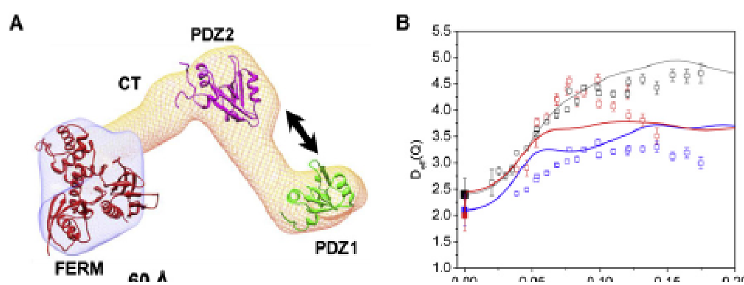




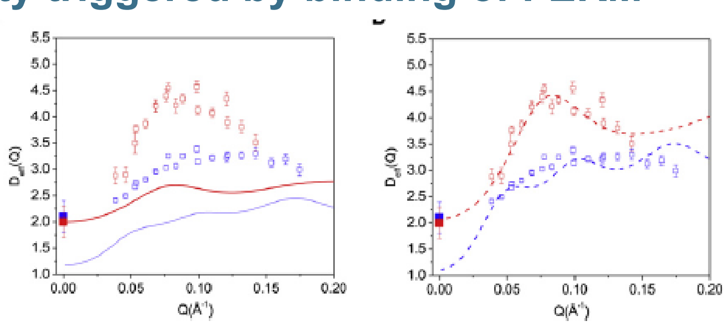
Inoue et al. BIOPHYS J. 99 (2010): 2309

Domain Motion in PDZ Scaffolding Protein

Farago et al. , Biophys J. 99, (2010) 3473



- Mobility triggered by binding of FERM



- Future possibilities

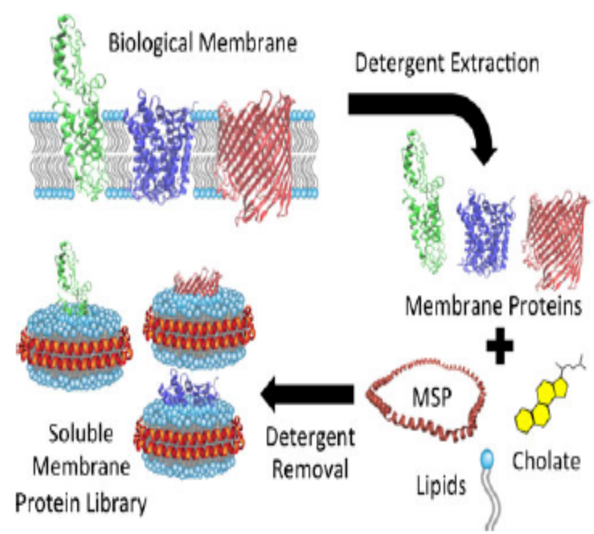
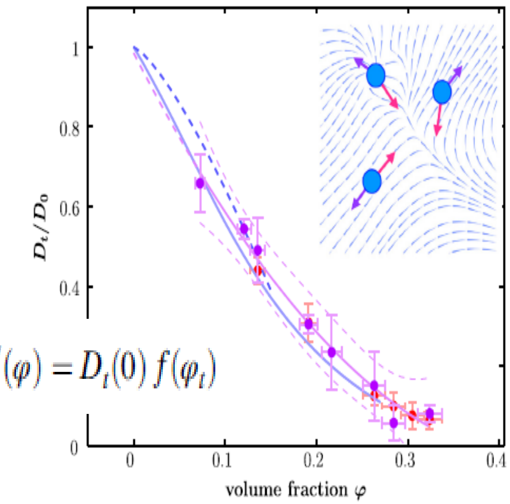


figure from: Marty et al. Anal. Bioanal. Chem (2013) 405, 4009

NSE-Science Case - complex fluids:

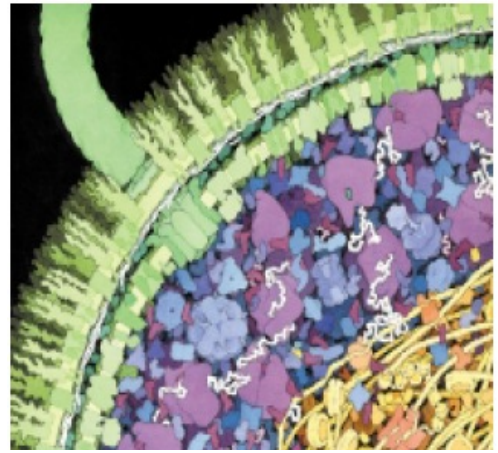
- Crowded (protein) solutions



$$D_t^{\mathrm{theory}}(\varphi) = D_t(0)\, f(\varphi_t)$$

Roosen-Runge et al. PNAS 108(2011)11815

- Crowding in a cell



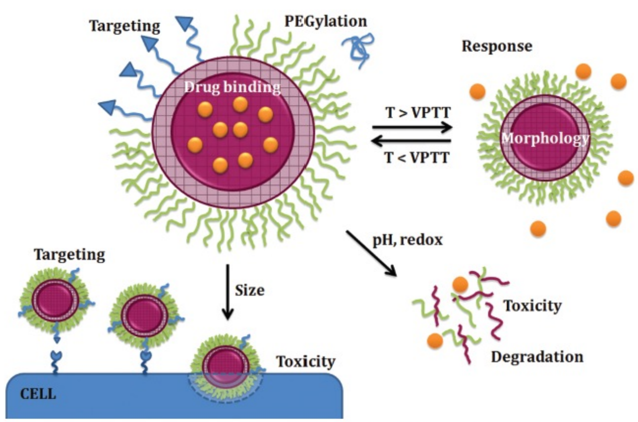
Hoppert, M. and Mayer, F. (1999) Prokaryotes. *Am. Sci.* 87, 518–525

diffusion in dense systems:

protein interactions :

enzyme reaction rates

- **Microgels** (responsive, T, pH sensitive)



SCHEME 2 Schematic representation of the key design aspects of microgels for drug delivery applications.

Smeets et al., JOURNAL OF POLYMER SCIENCE, PART A: POLYMER CHEMISTRY **2013**, *51*, 3027–3043

- Ionic liquids

- Microemulsions

(with supercritical fluids, CO_2)

- Polymer (aggregate) solutions

- Dendrimers

NSE-Science Case - more topics:

- Glass physics

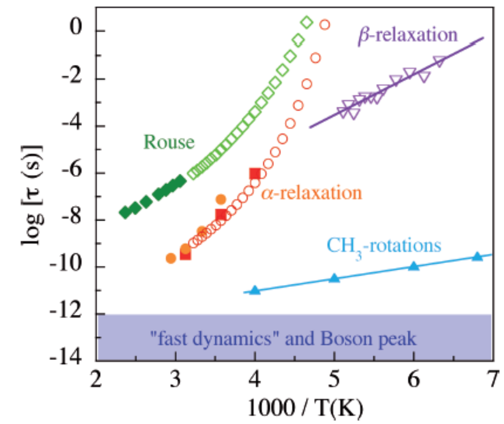
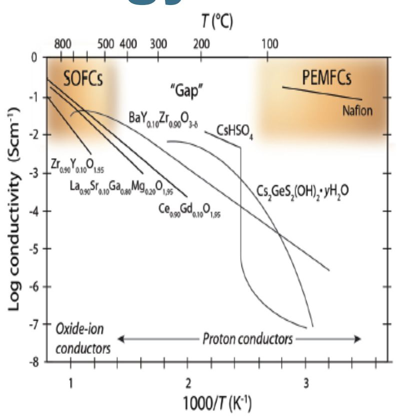
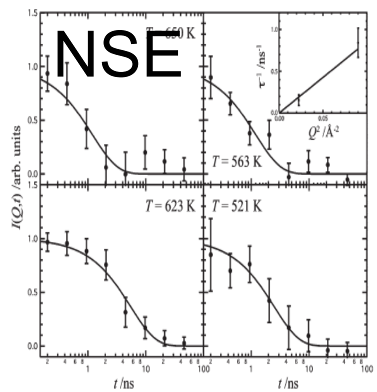


FIGURE 1 Relaxation map of polyisoprene. Full symbols corre- Arbe, Colmenero

- **Energy materials** – 1 electrolytes



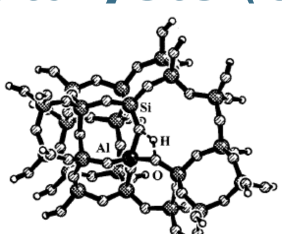


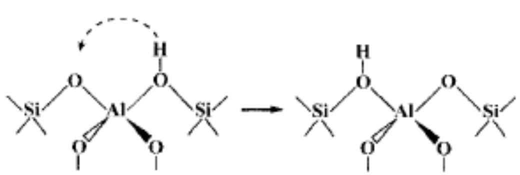
M. Karlsson

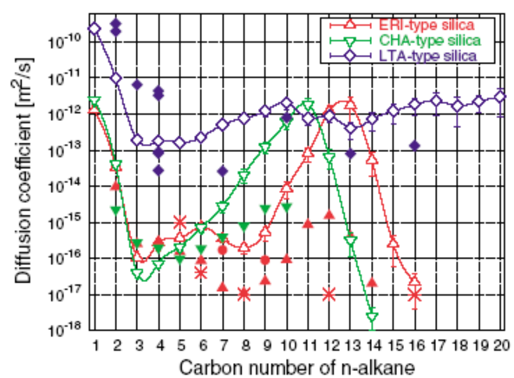
Dalton Trans., 2013, **42**, 317–329 | **317**

- **Energy materials** – 2 hydrogen storage

- **Catalysts** (e.g. molecular diffusion in zeolites, H. Jobic)







600 K

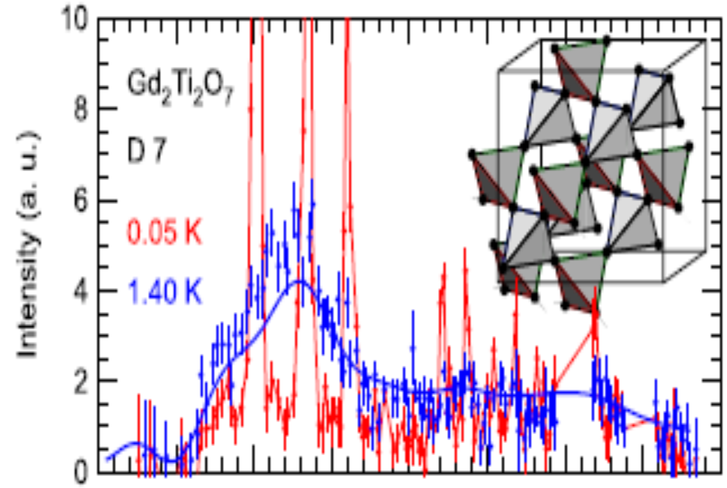
PRL **90** (2003) 245901

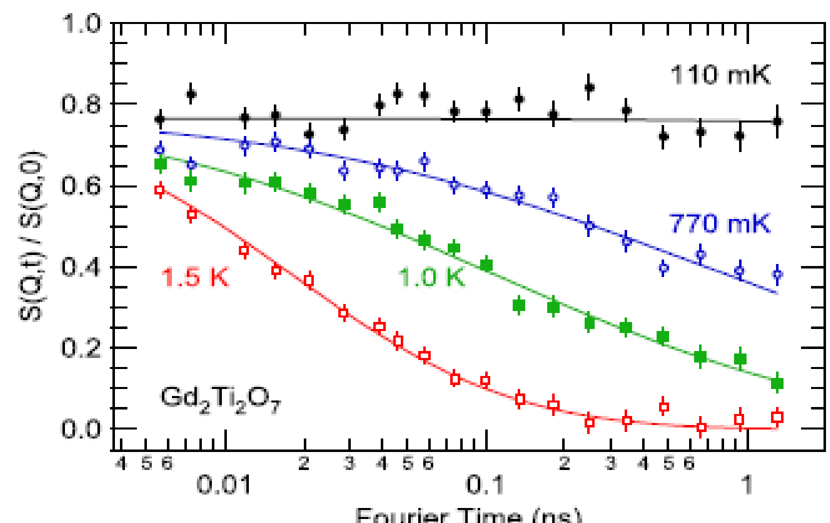
sim. to be tested by expt.

NSE-Science Case - magnetic:

- spin glass
- spin ice
- superparamgnetic fluctations
- geometrically frustrated magnets
- skyrmions (MnSi)

…





G. Ehlers

J. Phys.: Condens. Matter **18** (2006) R231–R244

High-Resolution NSE = large Fourier time

Max. Fourier time $\tau_{\max} = \begin{cases} \gamma J \dfrac{m_n^2}{h^2 2\pi} \lambda^3 \\ H\lambda^2 \end{cases}$

High flux (ESS)
and good polarization
@ long λ's

Large and homogeneous
(H) field integrals *(J)*

The High-Resolution NSE at ESS

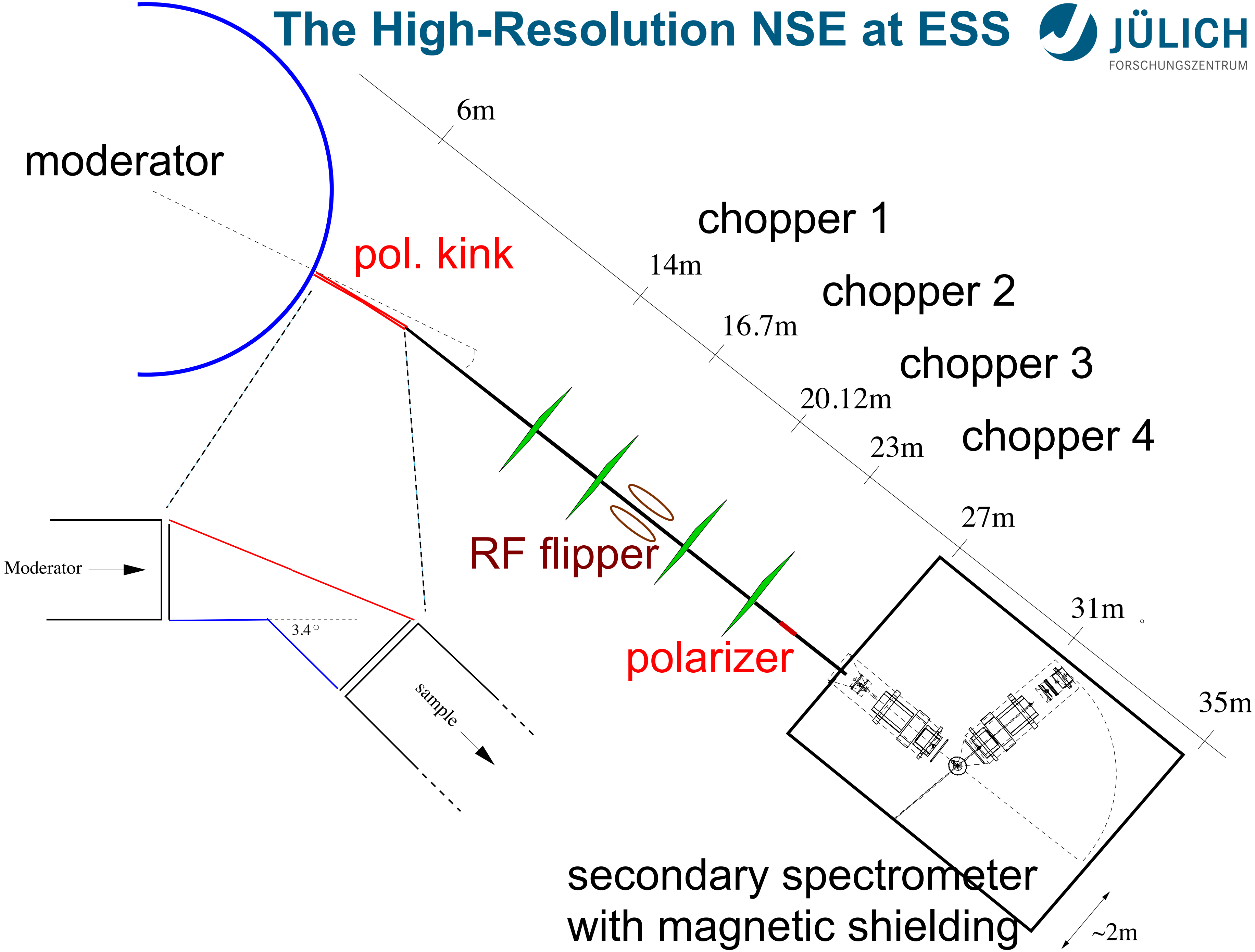
1) will be 35m long
   (if necessary extendable to 36m),

2) with a wavelength frame of 7÷8 Å,
   selected by 4 disk choppers

3) a Δλ/λ of 10% @ 3 Å,

4) and with two polarizers (FeSi) and a kink for
   an inclination of 3.4° from the direct line of sight.

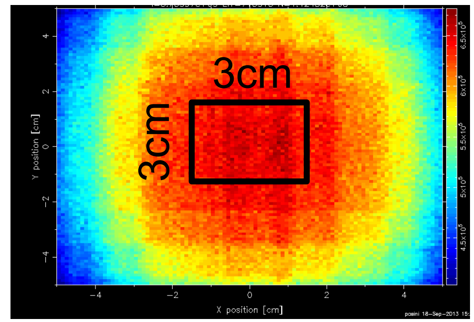
The High-Resolution NSE at ESS



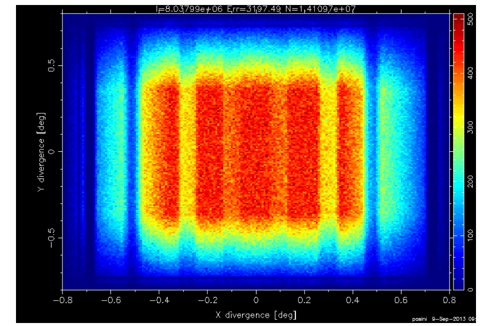
Beam extraction: performance at the sample

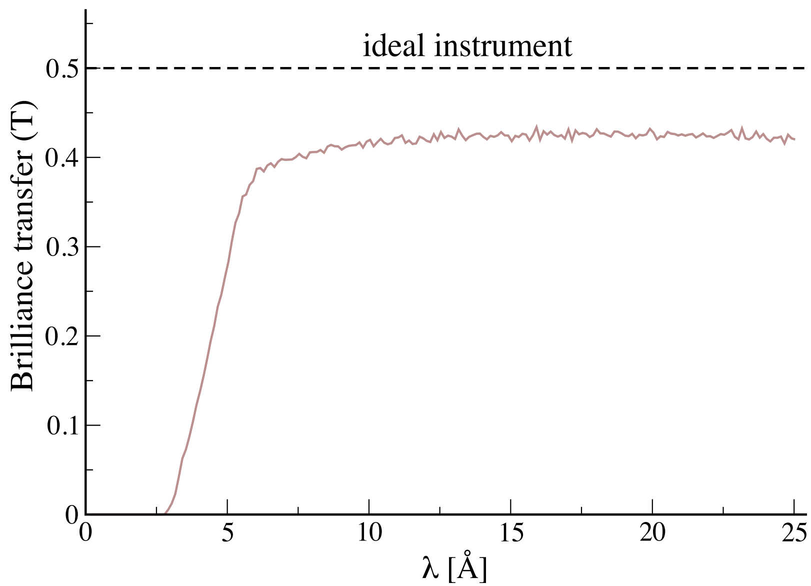
For a sample 3 x 3 cm^2 and @ 8 Å

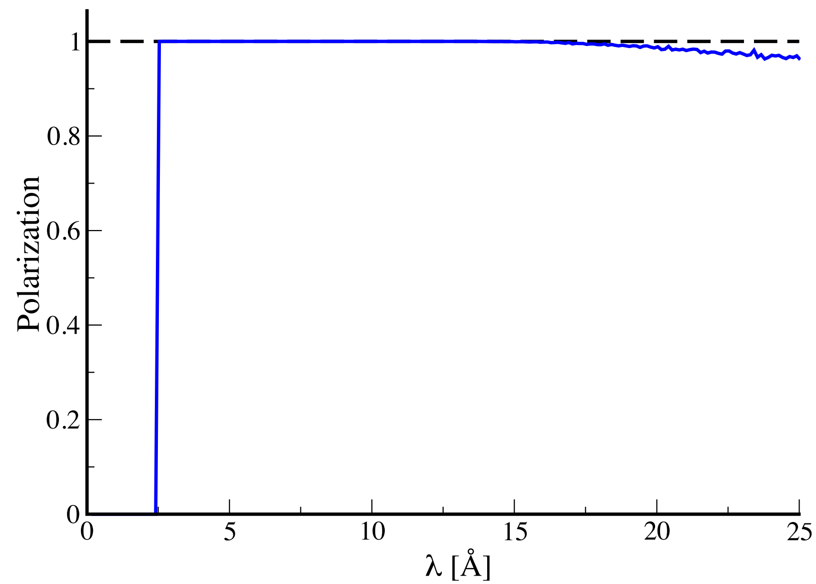
Position



Divergence



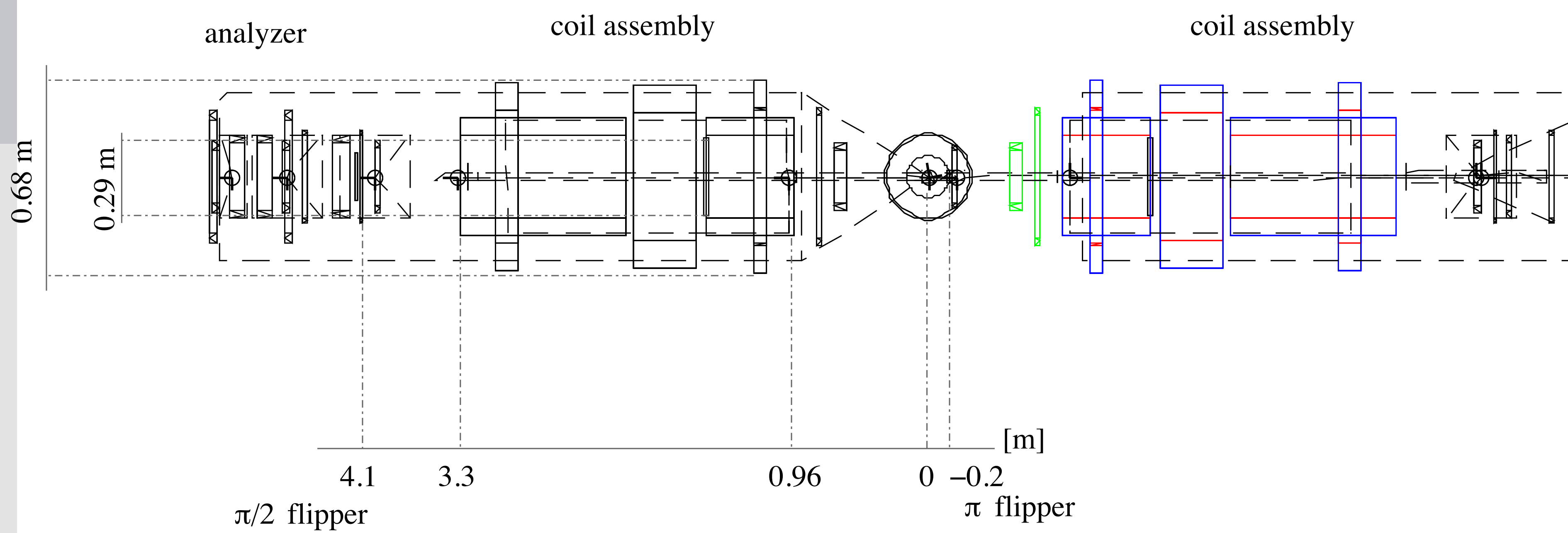




Improved design of magnetic coils

Superconducting coils
Fully compensated

Strategy ➔ Optimized coil geometry for maximally reduced field inhomogeneity



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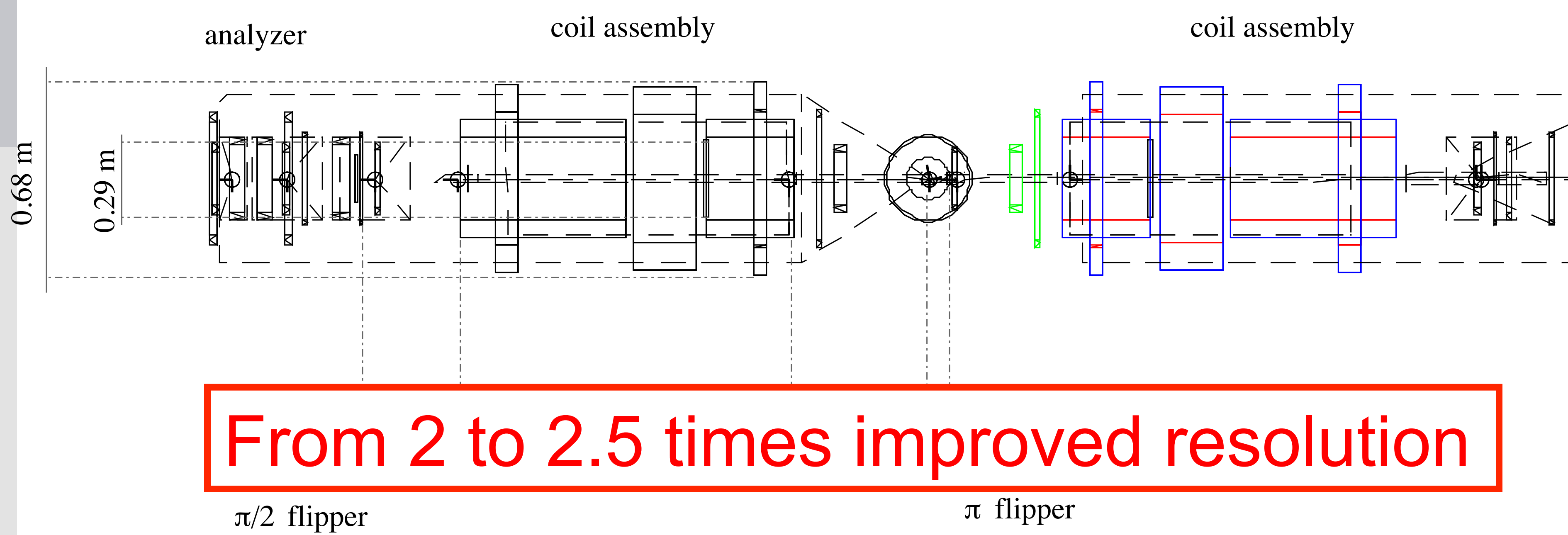

From 2 to 2.5 times improved resolution

Flux at the sample

λ	simulated Φ_{sample} [10^8 n/s/cm^2/Å]	Attenuation factors	Φ_{sample} ESS [10^8 n/s/cm^2/Å]	Φ_{sample} IN15 [10^8 n/s/cm^2/Å]	Gain ESS/IN15
6.3 Å	1.3	0.77 x 0.84 x 0.98	0.83	0.21	**3.9**
7 Å	0.9	0.76 x 0.81 x 0.97	0.54	0.18	**3.0**
17 Å	0.025	0.56 x 0.73 x 0.94	0.01	0.0035	**2.9**

For λ in [λ-0.5Å, λ+0.5Å], 4cm aluminium, 1m air and 5m He.

A factor 3 to 4 higher flux than IN15

→ larger guide section: 8cm x 8cm with m=2

Gain factors: Pulsed vs. continuous source

$$g = \frac{\ln\lambda_{max} - \ln\lambda_{min}}{w}, \text{ with } w = 0.15$$

$g \approx 5$ for λ in [7,14] Å or [8,16] Å

Flux at the sample

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A factor 3 to 4 higher flux than IN15

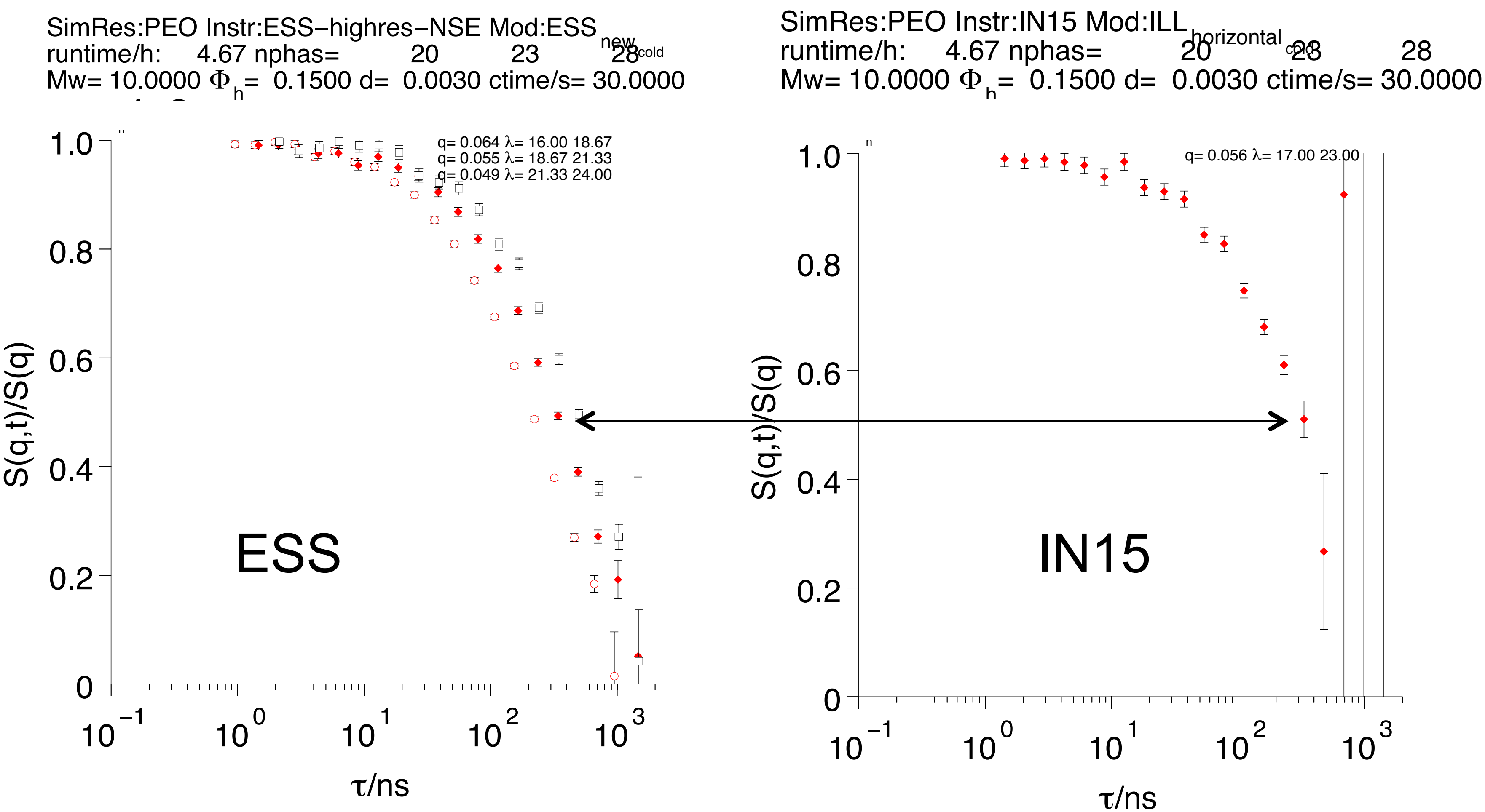
➔ larger guide section: 8cm x 8cm

Overall Gain Factor G = 15 ÷ 20

$g = \frac{\quad}{w}$, with $w = 0.15$

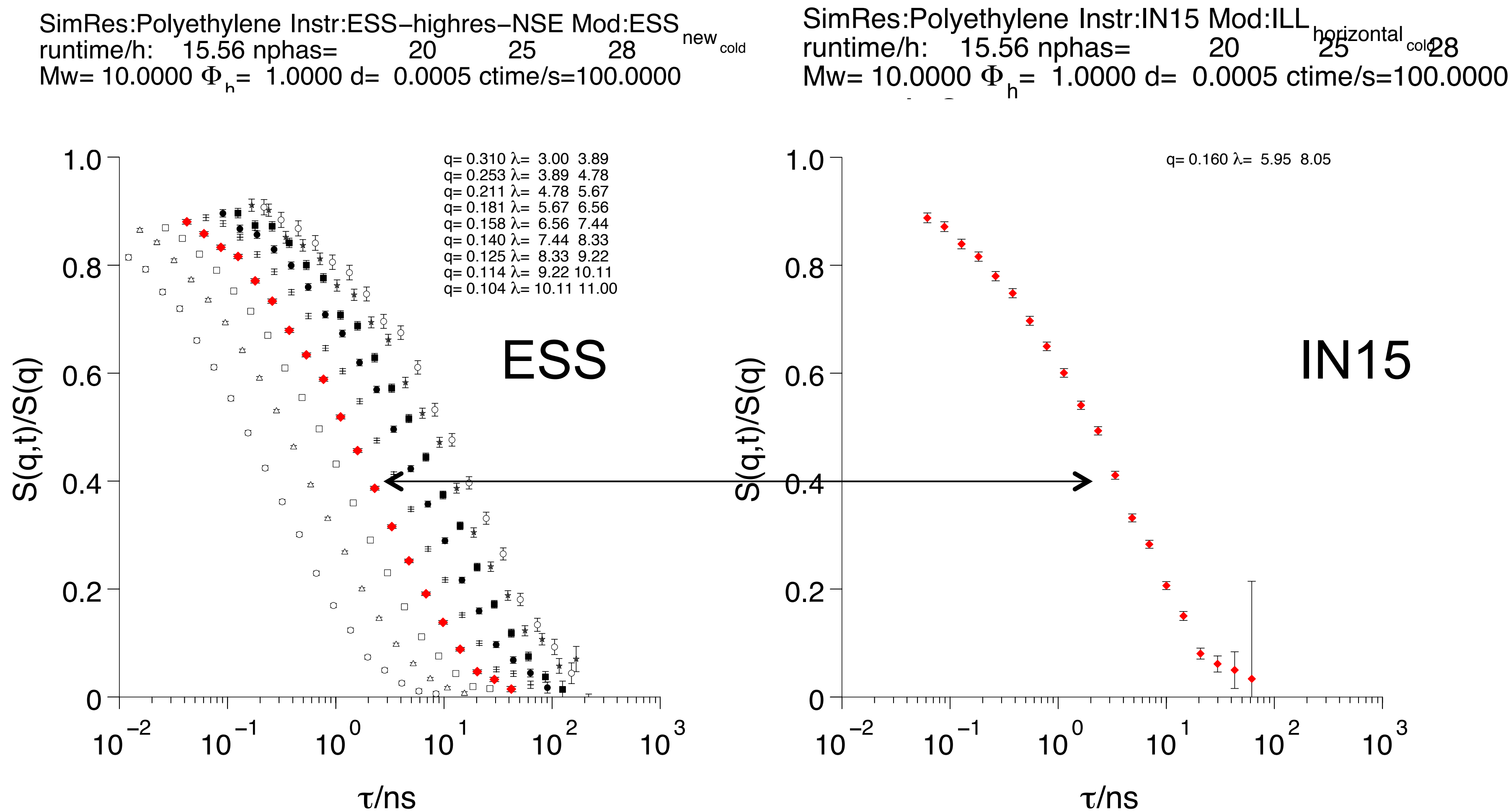
$g \approx 5$ for λ in [7,14] Å or [8,16] Å

ESS vs IN15
for polyethylene – simulated coh. scattering



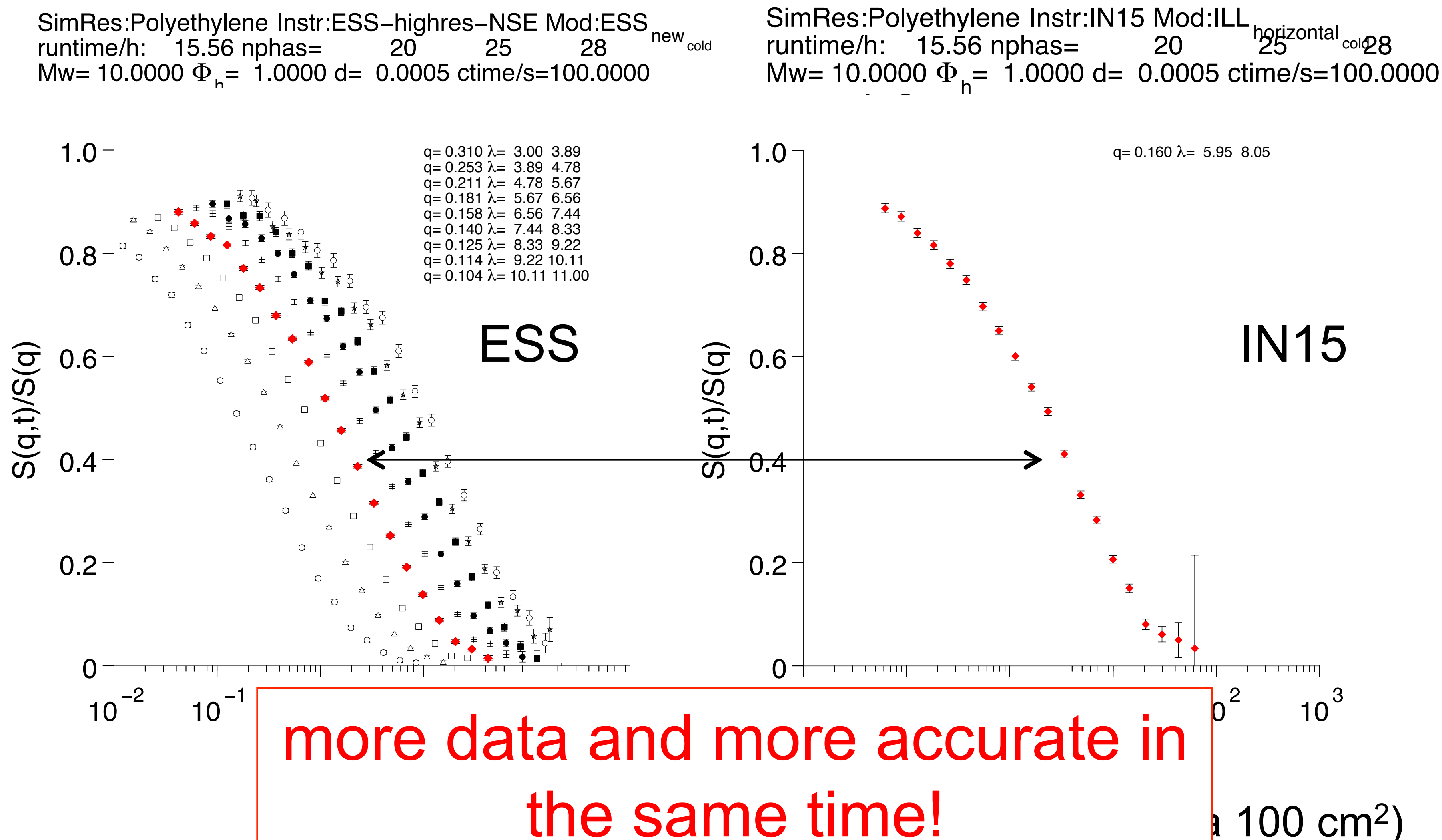
(Detector area 100 cm^2)

ESS vs IN15
for polyethylene – simulated incoh. scattering



(Detector area 100 cm^2)

ESS vs IN15
for polyethylene – simulated incoh. scattering



more data and more accurate in the same time!

THANK YOU!

Ionic liquids

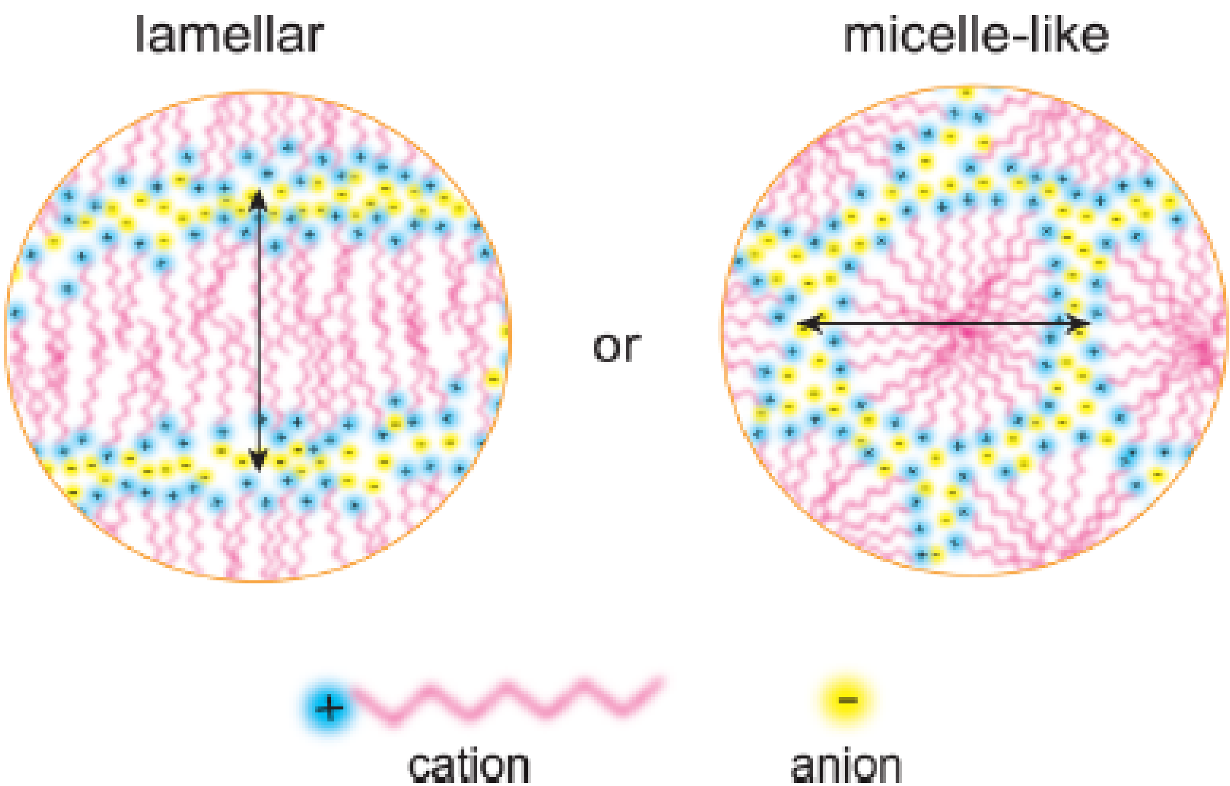


Figure 11. Schematic drawing of lamellar and micelle-like structure. The arrows correspond to the characteristic distance (~20 Å) of the low-Q peak.

dx.doi.org/10.1021/jp312608r | *J. Phys. Chem. B* 2013, 117, 2773−2781

The High-Resolution NSE at ESS

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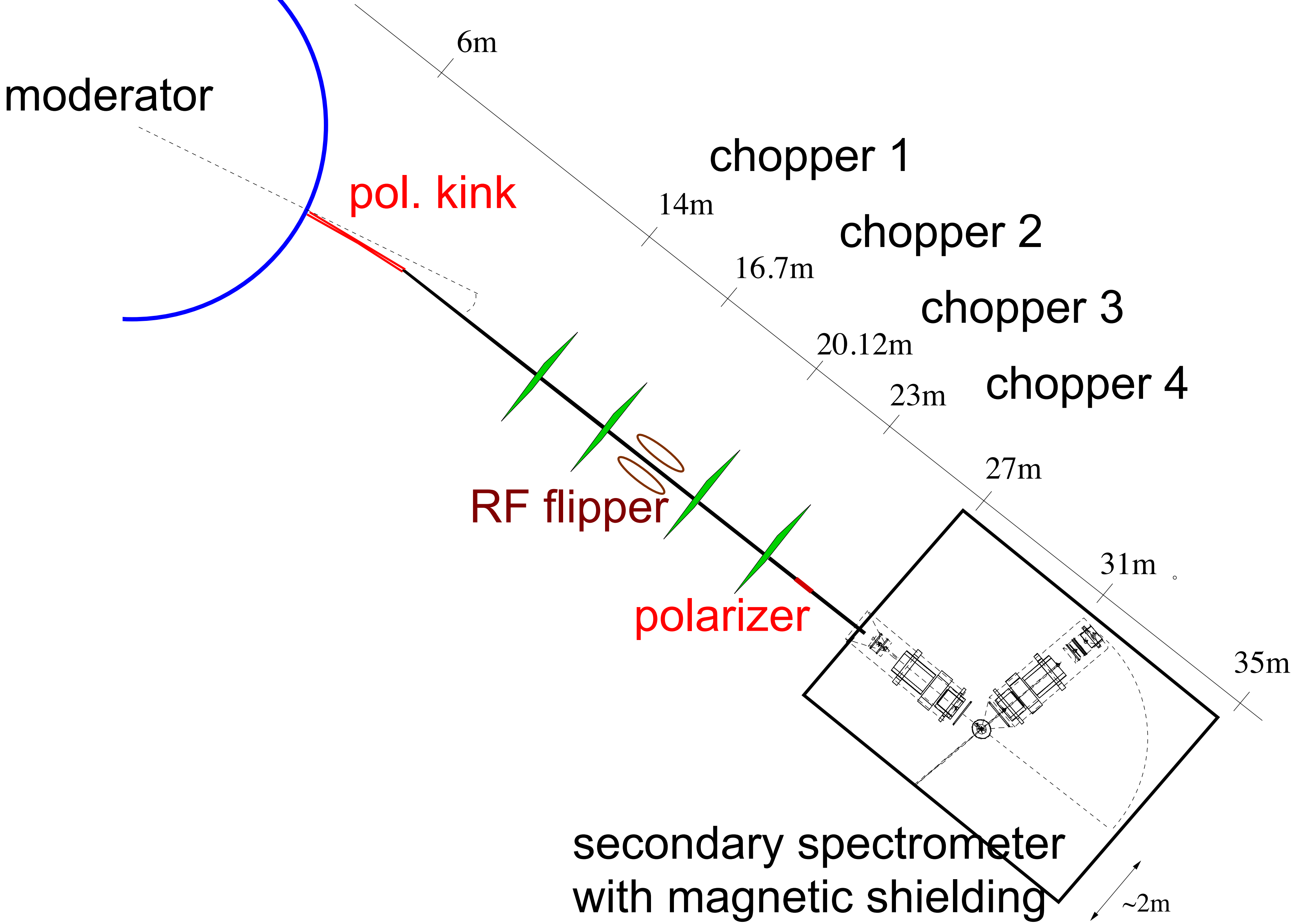
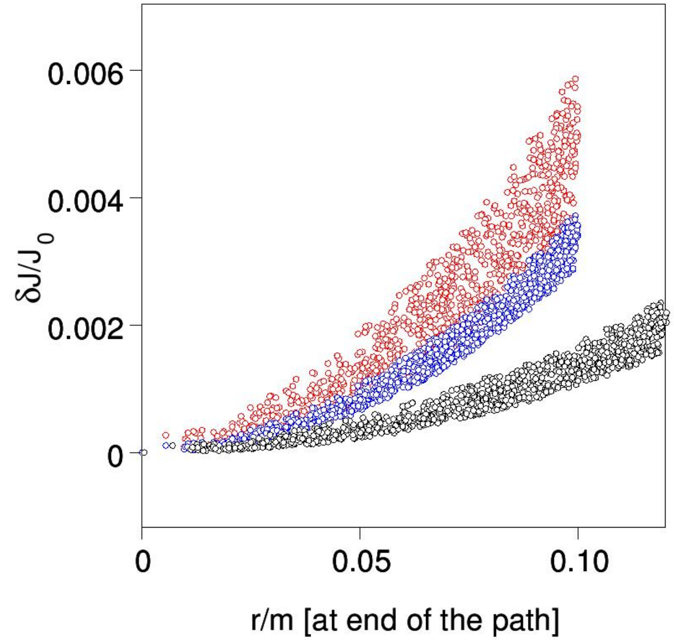


2÷2.5 times
Improved resolution



Inhomogeneity ~ 1ppm with only
2 (ideal) quadratic correction coils

(8Å, 100ns)	Current cc1	Current cc2	Current cc3
FRM2	44A	-14A	181A
SNS	78A	7A	184A
ESS	**44A**	**--**	**76-80A**

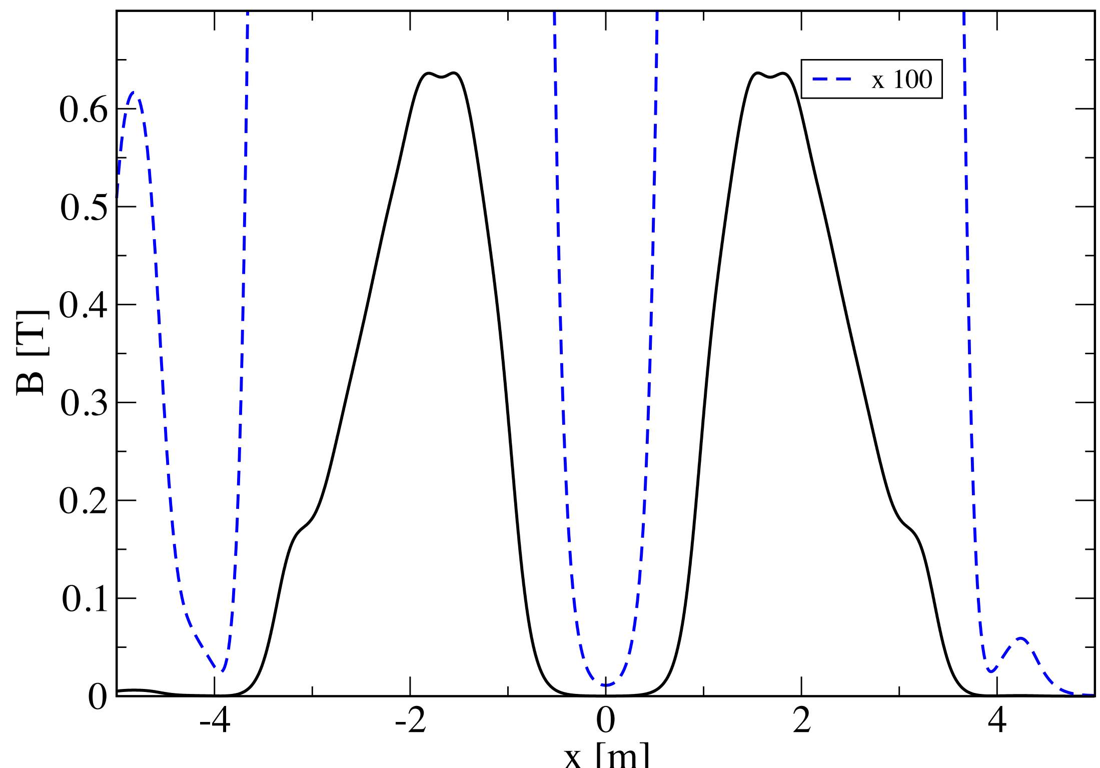
Super vs. normal conductors

- Higher field integral ➔ max J 1.5 – 2 Tm
- Experience from NSE @ SNS

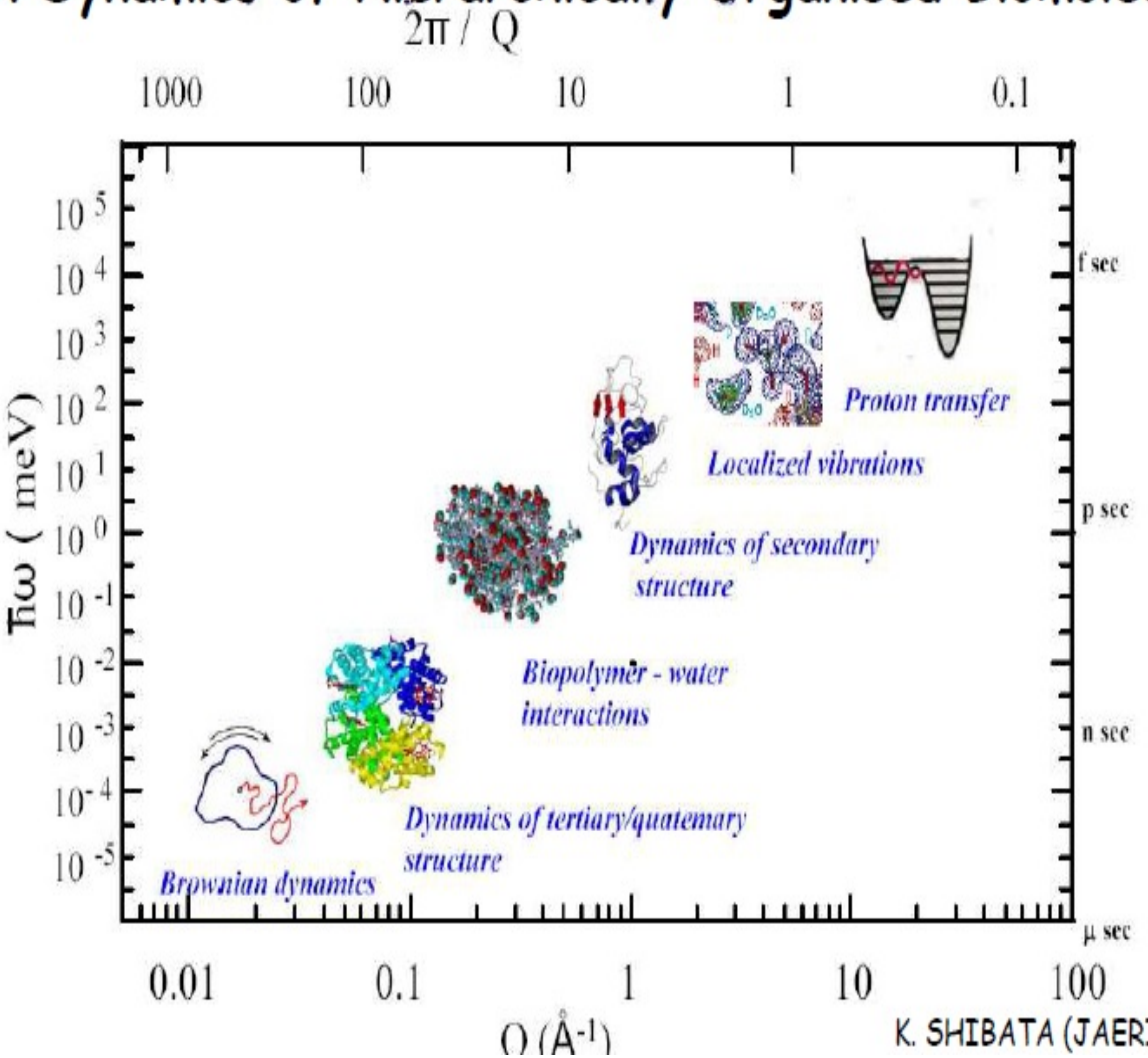
SNS ➔ for 0-1.8Tm **20min** for a complete scan (20 points)

➔ for 0-0.27Tm (IN15 max. range) **3min** for a complete scan

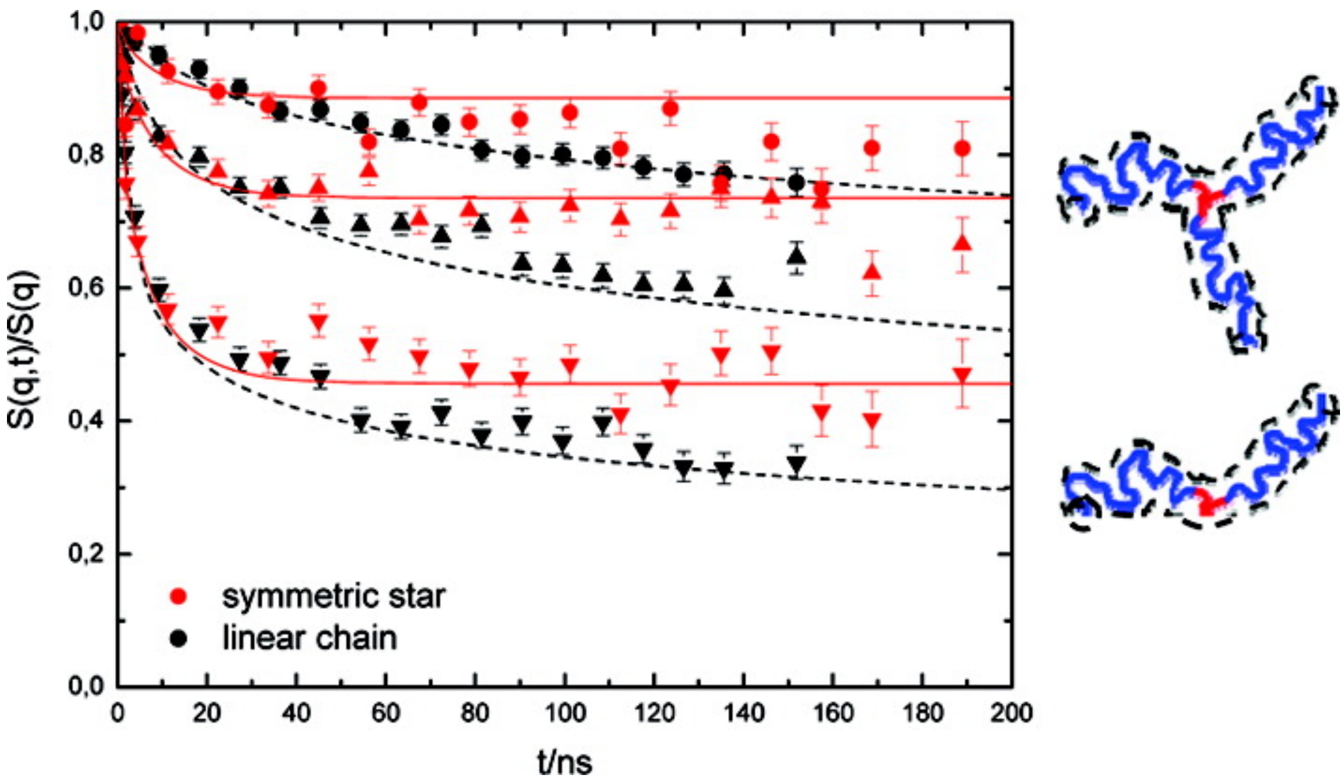
Field along the axis for both arms



The Rich Dynamics of Hierarchically Organised Biomolecules



K. SHIBATA (JAERI)



Published in: Michaela Zamponi; Wim Pyckhout-Hintzen; Andreas Wischnewski; Michael Monkenbusch; Lutz Willner; György Kali; Dieter Richter; *Macromolecules* **2010,** 43, 518-524.
DOI: 10.1021/ma9017185