Soft matter with polarised neutrons

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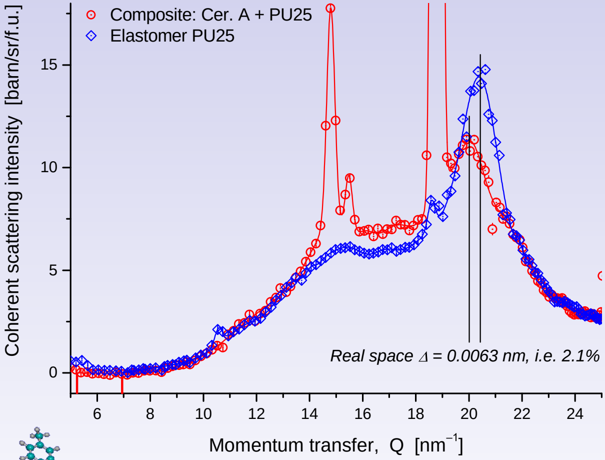
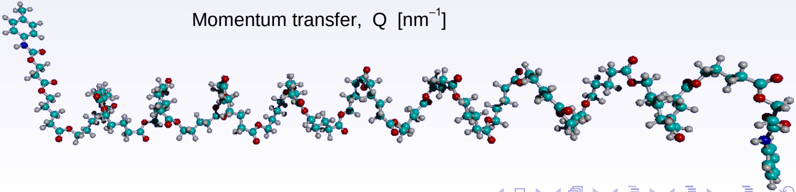
ESS Partner & Industry Day
Kraków, 25.03.2014

Residual strain in the PU–SiO_2 composite.
WANS spectra (polarised neutrons) for PU.



Peak at
$Q = 20.35\,\mathrm{nm}^{-1}$
most likely due to
Short Range Order in soft segments.



Neutron spin as a measuring probe

- Polarized neutrons offer a unique opportunity of separating, **at the machine level,** coherent from incoherent scattering. See how it works:
- If $\hat{B}\left(\vec{I}\cdot\vec{\sigma}\right)$ denotes the interaction operator between the neutron spin and the nuclear spin, then the following holds for the scattering intensity in the spin-flip and non-spin-flip channels:

$$I^{\uparrow\uparrow} = \frac{1}{3}\left|B\right|^2 \mathrm{I}\left(\mathrm{I}+1\right), \qquad \text{and} \qquad I^{\uparrow\downarrow} = \frac{2}{3}\left|B\right|^2 \mathrm{I}\left(\mathrm{I}+1\right)$$

Thus the outgoing scattering intensity from unpolarized nuclear spins is always one third without, and two thirds with flip of the neutron spin from the polarised beam. The coherent scattering I_{coh} and incoherent scattering I_{inc} are linearly related to the measured spin-flip and non-spin-flip scattering:

$$I^{\uparrow\downarrow}_{corr} = \frac{2}{3} I_{spin\ incoh} \qquad \text{and} \qquad I^{\uparrow\uparrow}_{corr} = I_{coh} + \frac{1}{3} I_{spin\ incoh} + I_{isotope\ incoh}$$

$$I_{coh} = I^{\uparrow\uparrow}_{corr} - \frac{1}{2} I^{\uparrow\downarrow}_{corr}, \qquad \text{and} \qquad I_{spin\ incoh} = \frac{3}{2} I^{\uparrow\downarrow}_{corr}$$

- Spin-ncoherent scattering always implies neutron spin-flip, while coherent contains a combination of both spin-flip and non-spin-flip events.

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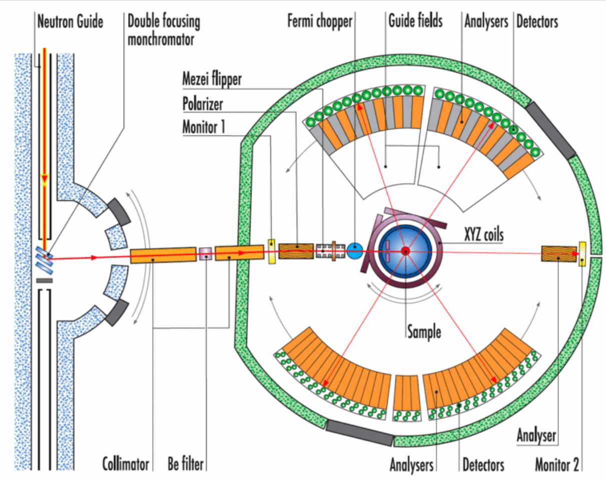
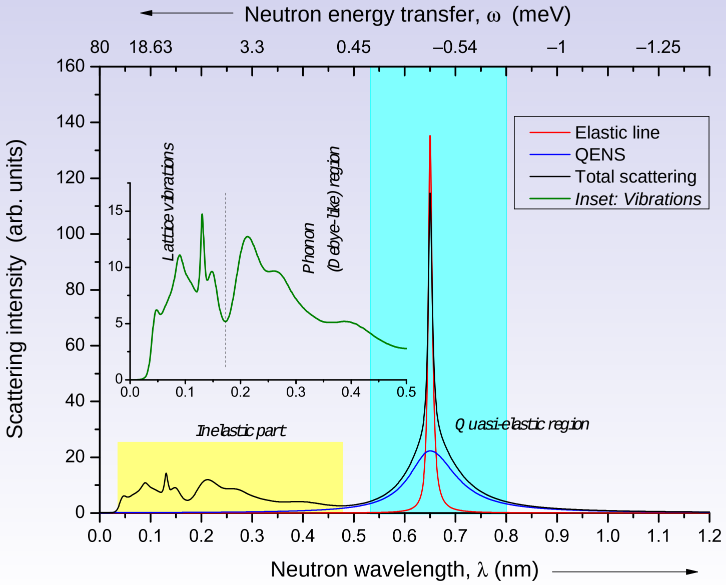
The instrument

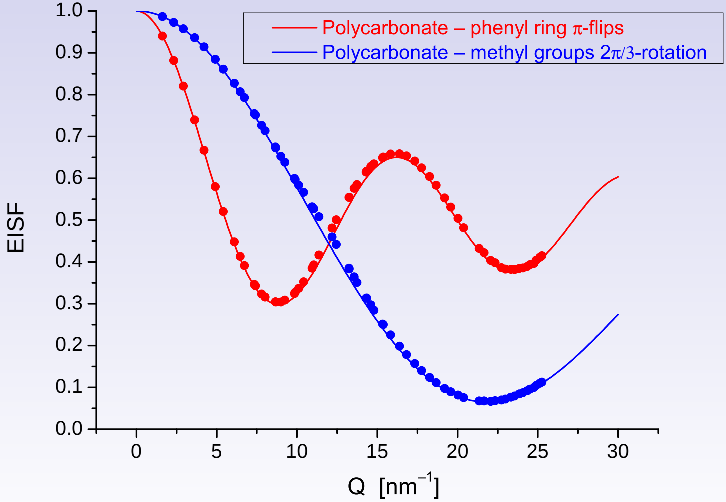
Such opportunity offers the D7 Diffuse Scattering instrument(ILL):



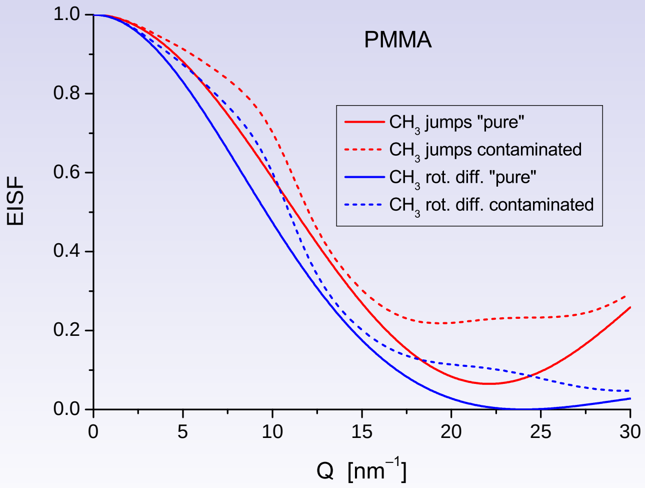
The INS/QENS spectrum "anatomy"



$\mathrm{EISF}(Q) = \dfrac{I_{el}(Q)}{I_{el}(Q) + I_{qel}(Q)}$ – an example



QENS on PMMA – an particularly nasty case of diffuse coherent scattering



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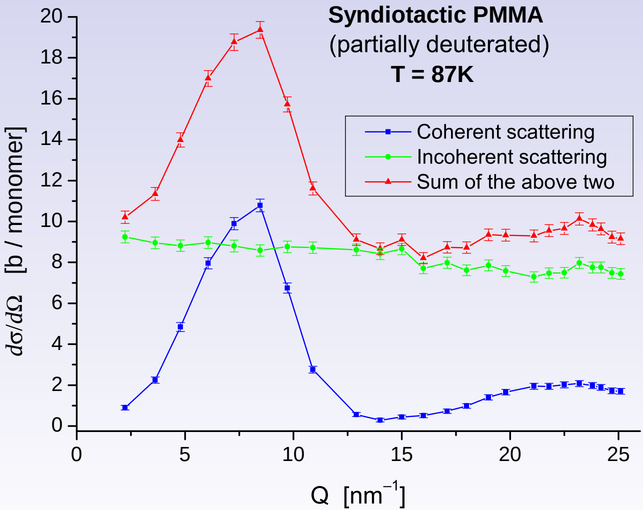
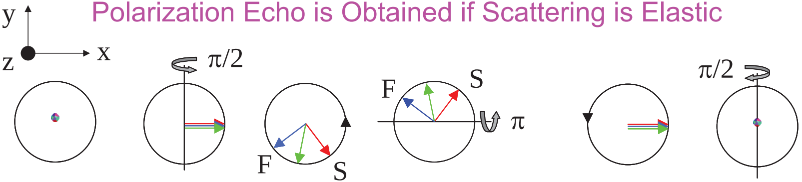


In NSE*, Neutron Spins Precess Before and After Scattering & a Polarization Echo is Obtained if Scattering is Elastic



Initially, neutrons are polarized along z

Rotate spins into x-y precession plane

Allow spins to precess around z: slower neutrons precess further over a fixed path-length

Rotate spins through π about x axis

Elastic Scattering Event

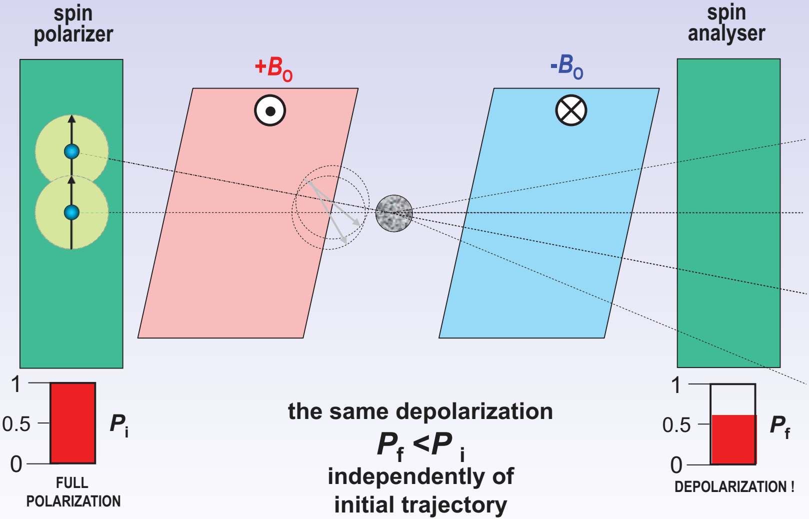
Allow spins to precess around z: all spins are in the same direction at the echo point if $\Delta E = 0$

Rotate spins to z and measure polarization

$$\textit{Final Polarization, } P = \langle \cos(\phi_1 - \phi_2) \rangle$$

* F. Mezei, Z. Physik, 255 (1972) 145

NSE principles

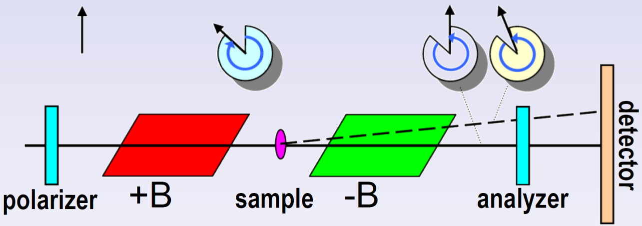


the same depolarization

$$P_f < P_i$$

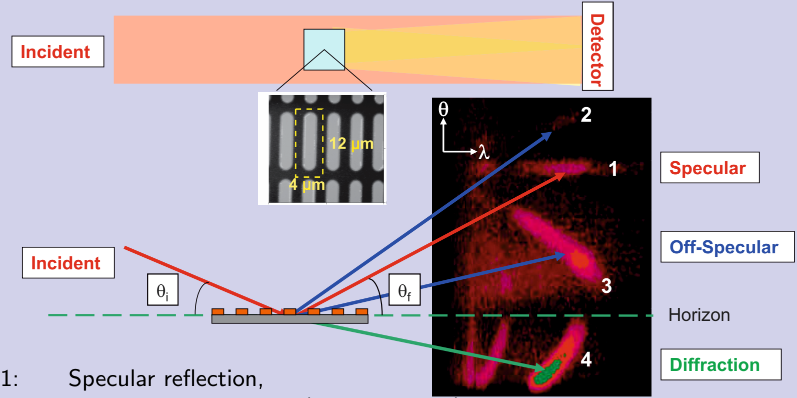
independently of initial trajectory

The principle of SESANS



SESANS, SERGIS

Spin Echo Small Angle Measurement (SESAME)
Spin Echo Resolved Grazing Incidence angle Scattering (SERGIS)



1: Specular reflection,

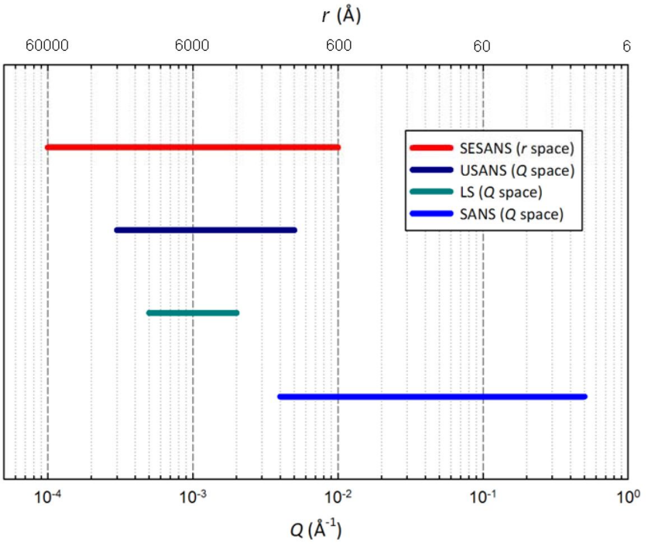
2, 3: Off-specular reflection (above horizon)

$$\theta = \theta_i + \sqrt{\theta_i^2 + 2n\lambda/d} \quad n = \pm 1$$

4: Off-specular diffraction (below horizon)

$$\theta = \theta_i + \sqrt{\theta_i^2 + 2n\lambda/d - Nb\lambda^2/\pi} \quad n = -1$$

Length scales probed by SESANS



(Wei-Ren Chen et al., "The Theoretical Foundation of Spin-Echo Small-Angle Neutron Scattering (SESANS) Applied in Colloidal System", UCANS-II Indiana University; July 08th 2011; Bloomington, IN)

Principles of Dynamic Nuclear Polarization

The scattering amplitude a of thermal neutron, carrying spin s; $\left(|\mathbf{s}| = \frac{1}{2}\right)$ interacting with a nucleus of spin $\mathbf{I}$ (Abragam, Goldman; 1982):

$$a = b + 2B\left(\mathbf{I} \cdot \mathbf{s}\right)$$

The constants b and B are determined by the two eigenvalues $b_{(+)}$ and $b_{(-)}$ of the operator $(\mathbf{I} \cdot \mathbf{s})$, depending on whether $\mathbf{I}$ and s couple in the channels $I + \frac{1}{2}$ or $I - \frac{1}{2}$. They may be interpreted as spin-independent and $\frac{1}{2}$ of spin-dependent scattering lengths:

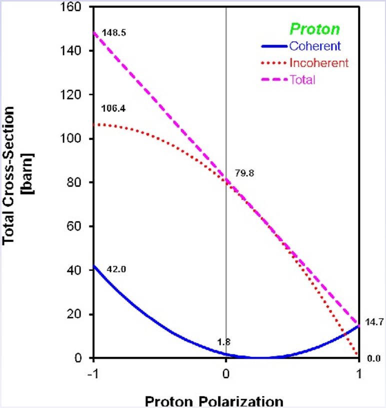
$$b = \frac{(I+1)\, b_{(+)} + I b_{(-)}}{2I+1}$$

$$B = \frac{b_{(+)} + b_{(-)}}{2I+1}$$

and for the hydrogen atom they are: $b = -3.74\,\mathrm{fm}$, $B = 29.1\,\mathrm{fm}$.

Principles of Dynamic Nuclear Polarization

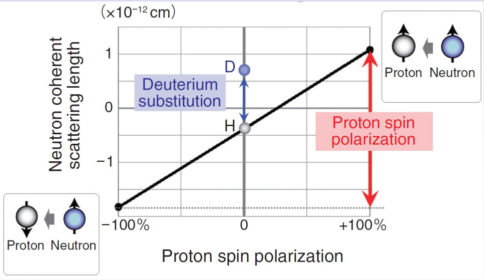
We assume a polarized target with polarisation, P_N, along an axis and the neutron beam polarized along the same axis with polarisation P_n. Furthermore, there are no correlations between the relative orientations of two nuclear spins and their relative positions in an unpolarized target. Then the total polarization-dependent coherent and incoherent neutron scattering cross-sections are:

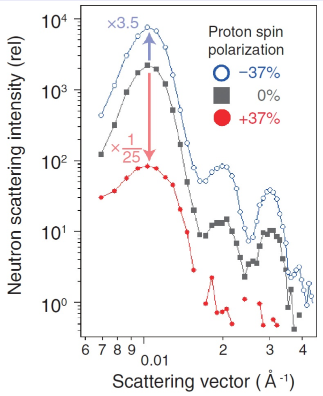


$$\sigma_{coh} = 4\pi \left[b^2 + P_n P_N \cdot 2IbB + P_N^2 I^2 B^2 \right]$$
$$\sigma_{inc} = 4\pi \left[I\left(I+1\right) B^2 - P_n P_N I B^2 - P_N^2 I^2 B^2 \right]$$

(J.H. Zhao et al, Physics Procedia **42** (2013) p.39-45)

Spin Contrast Variation





Small-angle neutron scattering (SANS) intensity decreased for positive spin polarization and increased for negative spin polarization. (Noda at al., J. Appl. Cryst. **44** 3 (2011) p.503-513)