IMAGING @ UNIVERSITY OF SOUTHERN DENMARK
INVITES FOR A WORKSHOP ON

ESS –

THE EUROPEAN SPALLATION SOURCE FOR ADVANCED MATERIALS SCIENCES
STATUS OF THE ESS, ITS FACILITIES, NEUTRON METHODS,
AND THE DANISH APPROACH TO PARTICIPATION

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Materials Sciences / Dynamics: the unique potential of neutrons for study of systems internal dynamics

Beate Klösgen: trying to substitute

so far:

study of **structure** by neutrons

in direct space	imaging / tomography
in inverse space	SANS, GISANS, diffraction,

another aspect: **dynamics** within a structure

- diffusion: lateral, rotational, hopping, …
- vibration: within molecules, within a lattice (phonons)
- fluctuation: uncorrelated motions (polymers, liquid crystals & sheets, …)

back to basics:
there are two mechanism to a wave to interact with matter

exchange of momentum or **exchange of energy**

(or exchange of momentum and energy)

elastic processes : Δp **inelastic** processes: ΔE

structure involves elastic processes

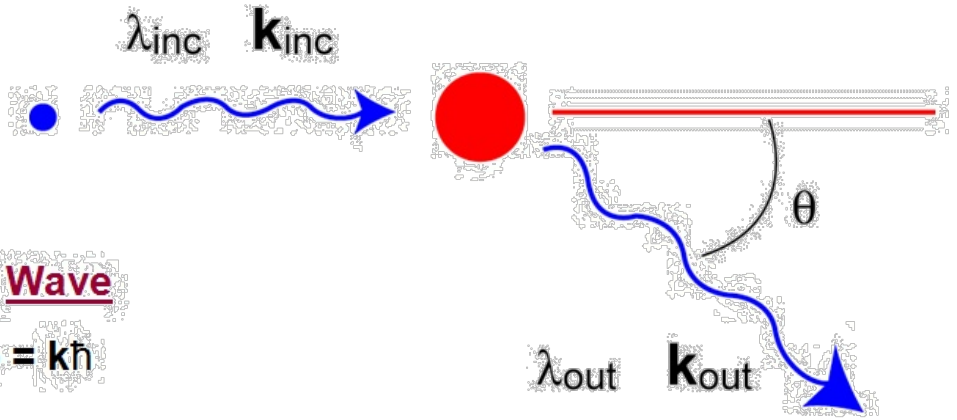
change of structure /fluctuation within structure related to **dynamics**
requires energy change / **involves inelastic processes**

structure studies
usually performed at **fixed energy** / wavelength

studies of **dynamics**
explore **change** of **energy** upon incidence of waves on matter

→ **spectrometer** needed behind the sample

Principles of neutron scattering



Particle

$E_{kin} = \frac{mV^2}{2}$

Wave

$\mathbf{p} = \mathbf{k}\hbar$

Scattering proces

$\hbar\omega = E_{out} - E_{inc} = \frac{m}{2}(V_{out}^2 - V_{inc}^2)$

$\mathbf{Q} = \mathbf{k}_{out} - \mathbf{k}_{inc}$

information about microscopic motion

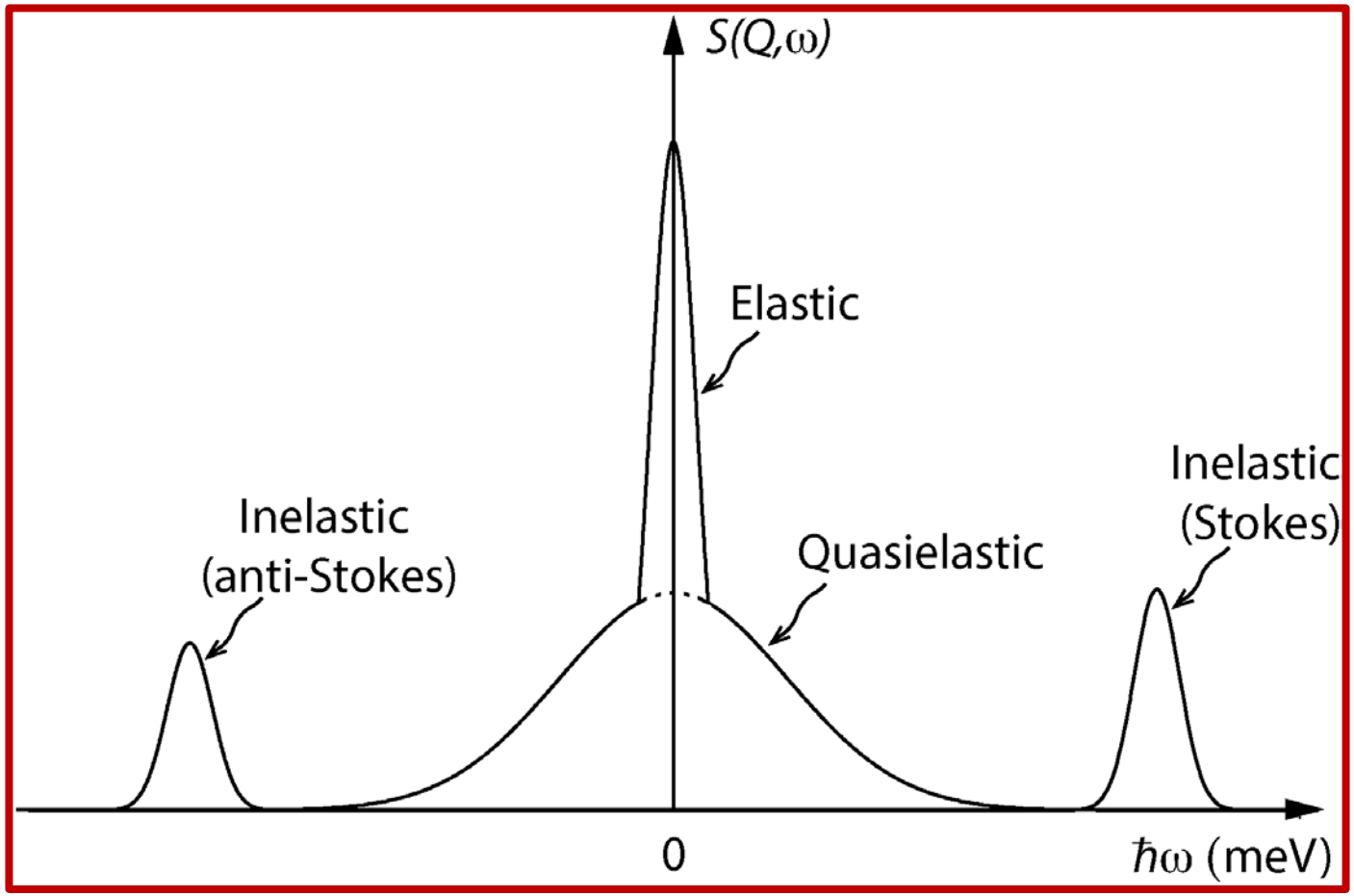
information about microscopic structure

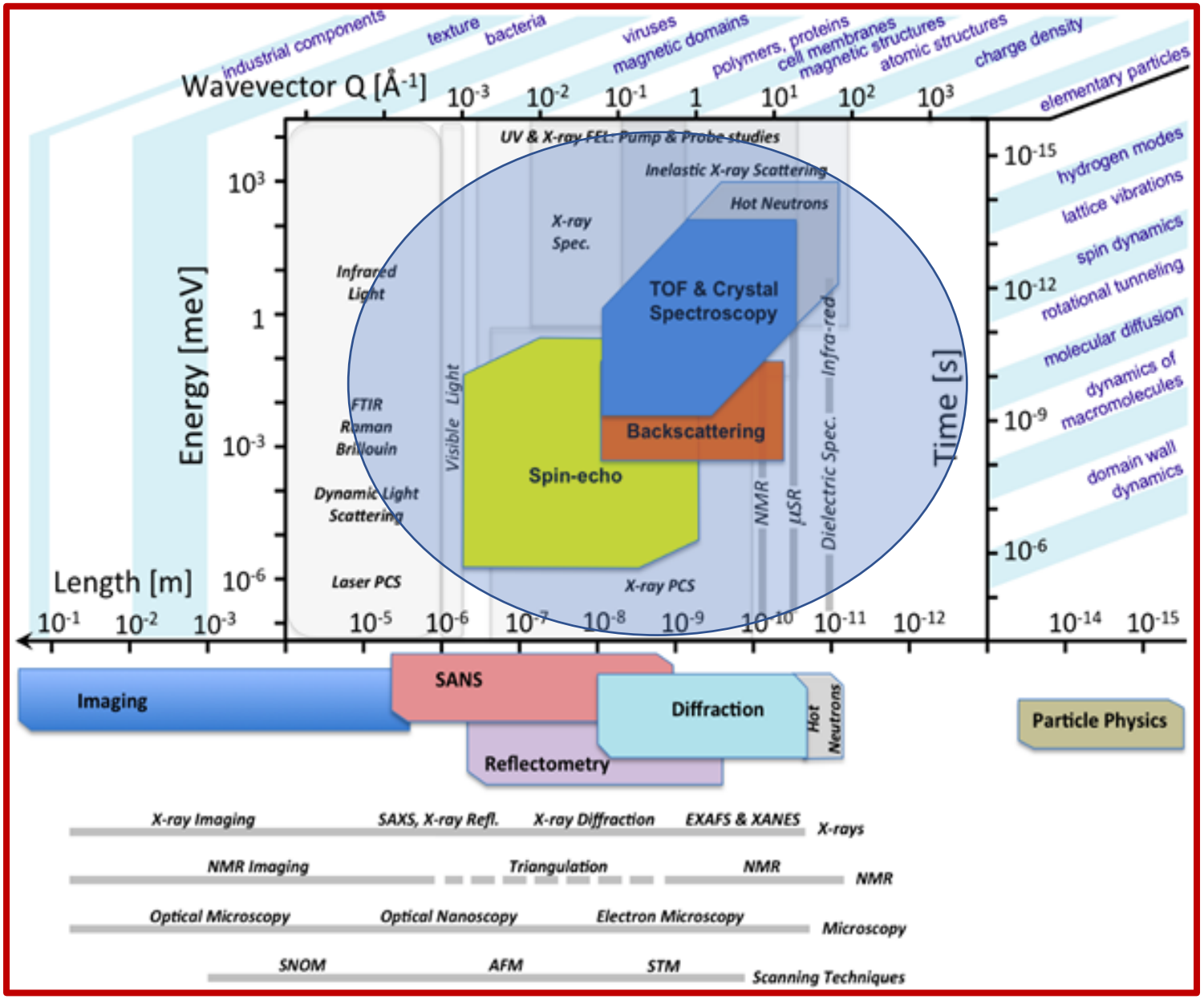
https://www.helmholtz-berlin.de/forschung/oe/em/softmatter/forschung/laufzeit/index_en.html

spectrometer measures distribution of energies I(E)

after **illumination** of a sample

with a beam of **well-defined narrow initial energy range (E_0+δE_0)**





https://europeanspallationsource.se/science-using-neutrons

types of spectrometers

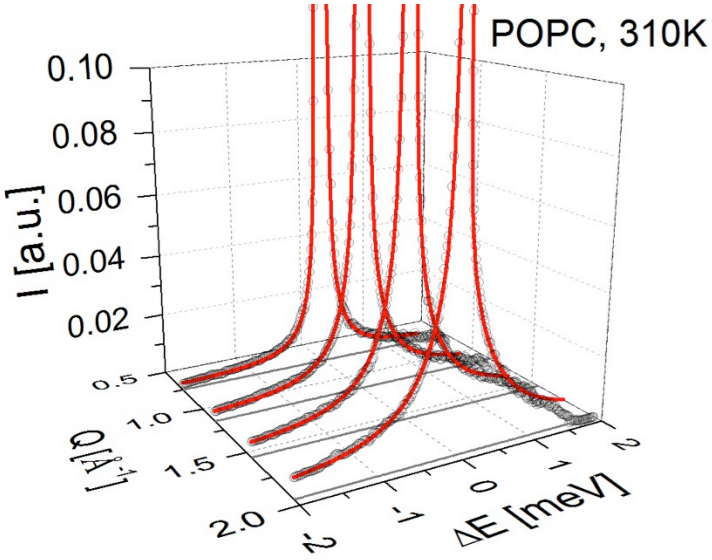
- time of flight
- backscattering
- spin-echo

new at ESS

- crystal focusing analyzers: **BIFROST** (Danish-Swiss)

examples:

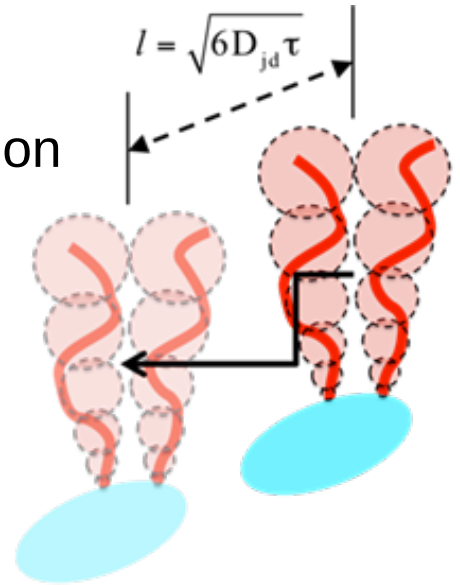
lipid in-plane dynamics , quasi-elastic incoherent neutron scattering (ILL@ IN13, IN5)



modelling of data:
two modes

- **restricted diffusion** (rd)
  for motions of intramolecular nuclei

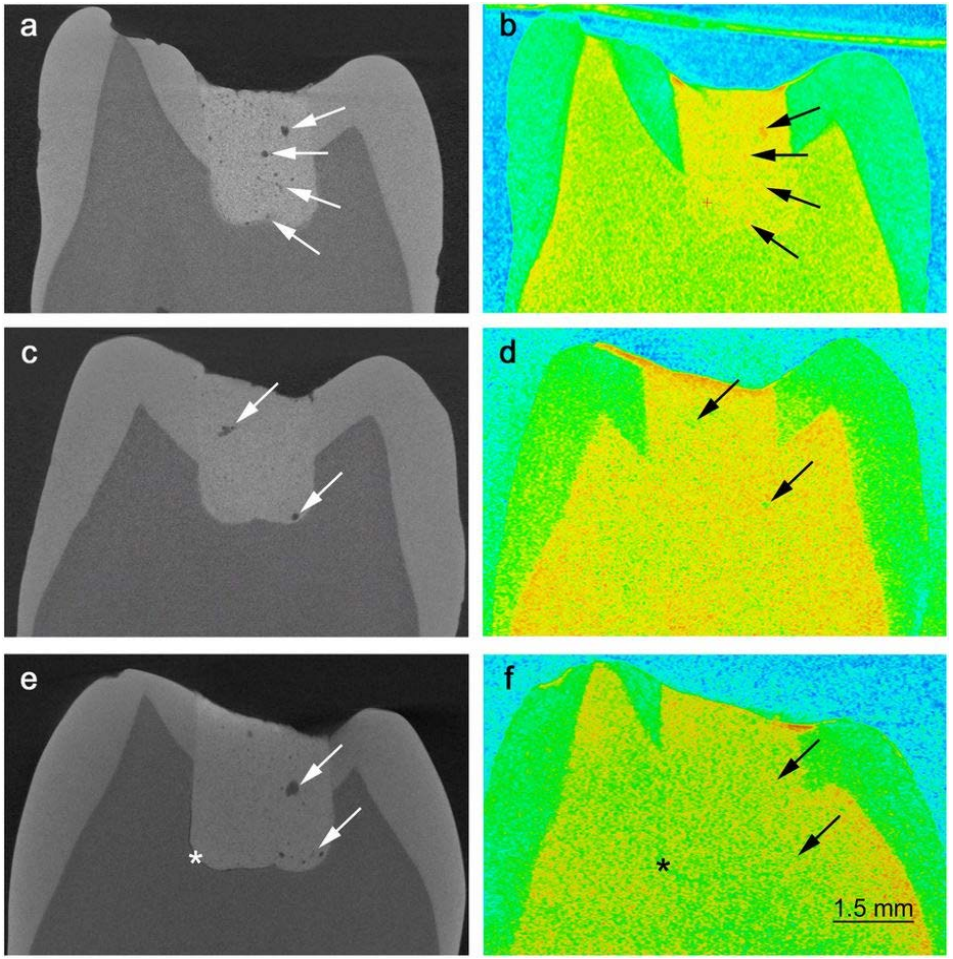
- **jump diffusion** (jd)
  for in-plane molecular motion



(Chen Shen, B. Klösgen, J. Peters, J.Pieper)

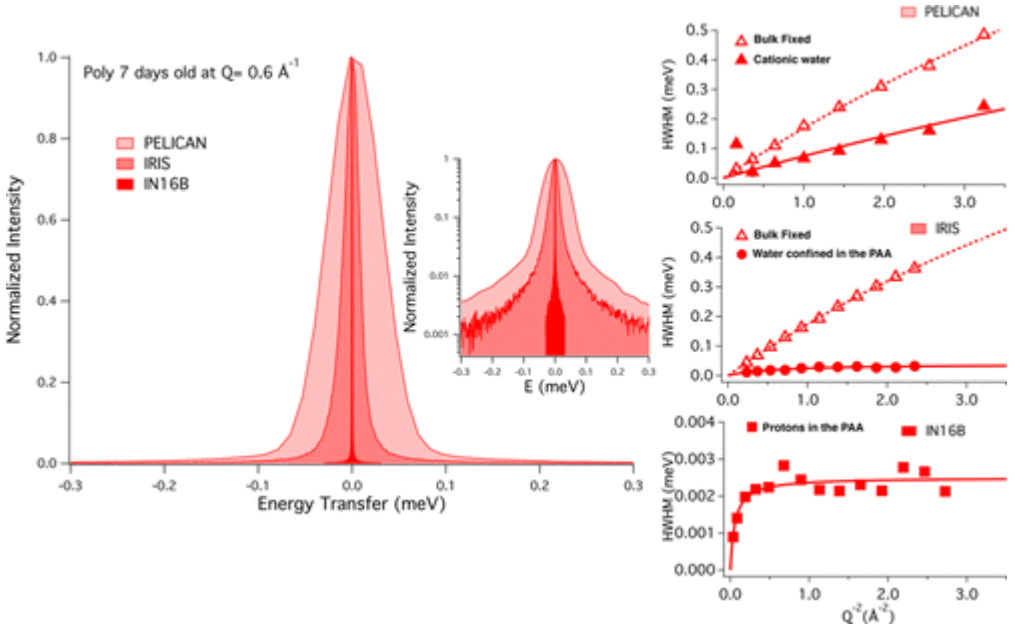
examples:

water hydrogene dynamics in teeth dental cements,
neutron tomography , quasi-elastic incoherent neutron scattering



x-rays:
cracks etc. well exposed

neutrons:
lower resolution,
but presence of liquid water suggested



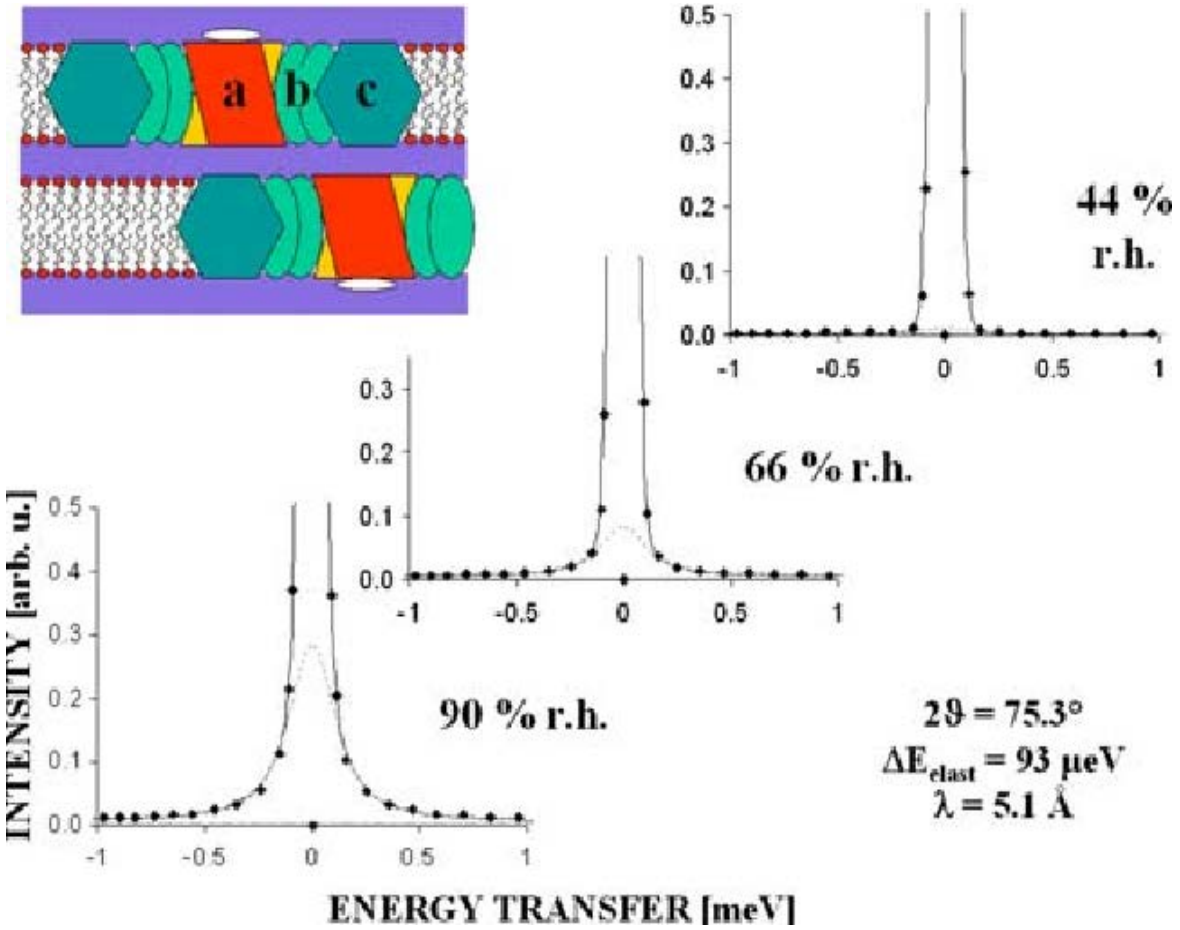
analysis improves understanding on

- **polymer–water** binding
- **polymer cross-linking**
- material **density** changes

(A. Benetti; H. Bordallo et al.)

examples:

hydrogene QENS for the study of protein dynamics,
neutron tomography , quasi-elastic incoherent neutron scattering



(Photosynthesis Research, 102, 281, 2009)

photosystem II (PSII)
in **membrane matrix**
humidity dependency uncovers

- **activation** of protein depending on matrix fluidity
- access to **photocycle states** by pump-probe technique coupled to QENS

(J. Pieper, G. Renger)

examples: ……

thank you for listening!

take home message on dynamic studies with neutrons

- neutron studies give information about **structure and dynamics**
- dynamic studies report on **mobility** of (hydrogen) nuclei in a system
- **different states** are distinguishable within a structure:
  solid, slow motions, fast motions, ….
- **tracer-free** diffusion studies are applicable
- **process / state models** are **experimentally accessible** / distinguishable
  - diffusion types: continuous, hop-diffusion, wall migration, …
  - **density distributions** along molecular and non-molecular interfaces (“wetting”)
  - **fluctuations** can be identified and classified
    (conformational states in polymer melts, transient dynamic states within proteins,
    undulations of liquid surfaces / interfaces, ….)