The Abdus Salam
International Centre for Theoretical Physics

United Nations
Educational, Scientific and
Cultural Organization

IAEA
International Atomic Energy Agency

1866-11

School on Pulsed Neutrons: Characterization of Materials

15 - 26 October 2007

Materials and Life Sciences at Spallation Neutron Sources (2)

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Kurt N Clausen PSI Switzerland

IAEA School on Pulsed Neutrons:

Characterization of Materials

Outline -----

Structural Biology

- The technique of choise / workhorse is Synchrotron X-rays
- How can neutrons play a role?

Neutrons

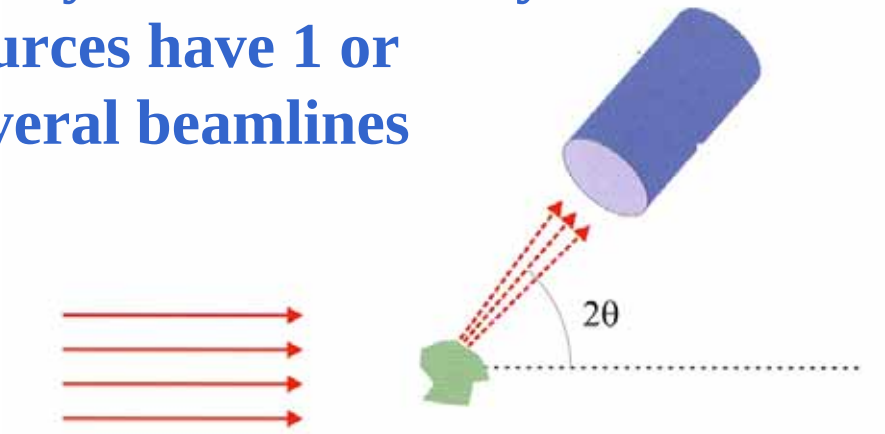
- Contrast matching – Solution scattering
- Finding H by neutron diffraction
- Reflectometry - Membranes
- Protein un-folding
- Colloids under shear,

Muon spectroscopy

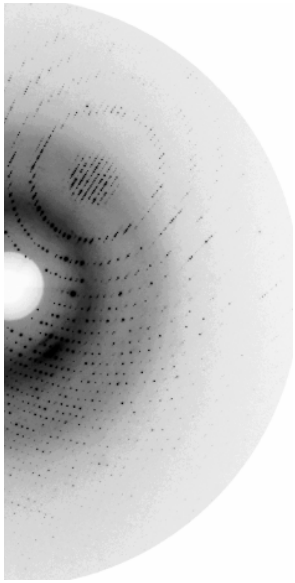
- Avoided Level Crossing – Detergent which looks and smells nice

Structural biology

All Synchrotron X-ray sources have 1 or several beamlines



X-ray beam

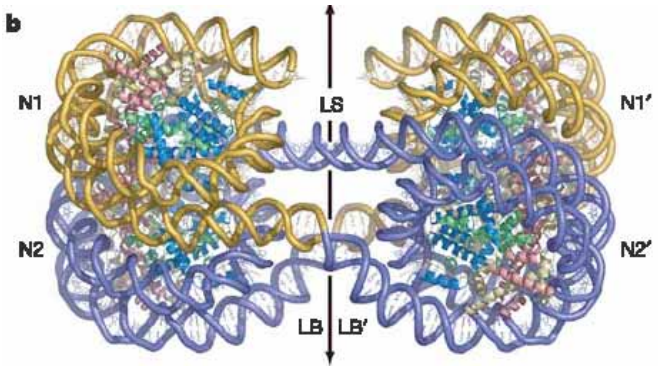


Diffraction pattern

The method of choise – X-rays but

ILL, LANSCE and JRR Japan has active groups

Structure of tetra-nucleosome
T. Richmond, ETH-Zürich
Marcel-Benoit Prize 2006



Protein crystallography with neutrons – problem:

Intensity

Intensity

and

Intensity – need for "huge" ~mm size single crystals

The first instrument suite at SNS – No protein crystallography, No dedicated Biology instruments! (SANS, Reflectometers and general spectrometers available)

JSNS is later and has protein crystallography in its first suite of instruments

Initiatives to change the situation at SNS is on the way.

	Crystallography			NMR	Cryo-EM	Solution scattering		Reflectometry
	X-rays	Electrons	Neutrons			SAXS	SANS	
Sample state	Small crystals (10^{-3} mm^3)	2D crystals (10^{-6} mm^2)	Large crystals (1mm^3)	Solution (0.5 ml, ~1mM)	Frozen in vitreous ice	Solution (0.02 ml, 0.1 mM)	Solution (0.2 ml, 0.1 mM)	Monolayer, few cm^2
Observed atoms	Heavy atoms, C,N,O,S,P, metals	Potential function	All atoms, incl. H/D	protons	No atomic resolution	No atomic resolution	No atomic resolution	No atomic resolution
Resolution	0.5 – 3 Å, typically 2.2 Å	2 – 10 Å	1.5 – 10 Å	~1Å RMSD	>20 - 30Å	Shape and distances	Shape and distances	Shape and distances
Structures in data bases*	12,796	~5	9	2,394	n.a.	n.a.	n.a.	n.a.
Size limit	None	None	<30kDa	<30-40kD	None	None	None	None
Strengths	High resolution, large assemblies	Direct phase information, 2D-crystals, membrane proteins	H-bonding, hydration, hydrogens in metal sites	Dynamics, binding, hydrogens	Large assemblies	Shape, some orientation	Orientation, shape, multi-component analysis, contrast variation	Membrane systems, contrast variation

*Protein Database, 25th July 2001

2006 first structure 50 kDa (ILL)

Different Methods
in the Comparison

Extract from

Report on Neutrons in Biology Workshop
Australian Institute for Nuclear Science and Engineering
School of Biochemistry & Molecular Biology, University of Melbourne
Australian Nuclear Science and Technology Organisation (ANSTO)
10-11 July 2001

NEUTRON SCATTERING & THE LIFE SCIENCES *Extracted from: "Neutron Scattering and the Life Sciences. A Strategy for the ILL" by P. A. Timmins*

Some notable cases (resent – a few years old) in which material was not a major problem and important contributions were made using neutron techniques, in almost all cases through exploitation of deuterium labelling either of the molecule or its aqueous solvent.

- The localisation of glycolipids and the translocation pathway in purple membrane
- The binding of detergent to membrane proteins
- The first studies of pico-second dynamics in proteins.
- The quaternary structure of the nucleosome, where neutron scattering was the first technique to demonstrate that the DNA was wound on the outside of the histones
- The ribosome, where all 21 proteins of the 30S sub-unit were placed by neutron triangulation of labelled sub-units produced *by in vivo* deuteration. This work is now proving invaluable in the interpretation of the high-resolution X-ray maps .
- The identification of the active site proton in trypsin, which allowed the mechanism of action of this enzyme to be understood.

What are the biological systems amenable to study and which are the techniques most likely to be of use in the Life Sciences?

NEUTRONS WILL NOT BE A KEY TOOL – DO NOT COPY THE SUCCESSES OF X-RAYS OR NMR – LOOK AT WHERE NEUTRONS ARE COMPLEMENTARY

The contribution of neutrons to Life Sciences will be on a wide front

- in macromolecular crystallography,
- small-angle scattering from large non-crystallisable systems,
- fibre diffraction,
- reflectometry and wide angle diffraction from natural and model membranes
- inelastic scattering for macromolecular dynamics.

Neutron crystallography

- is the only neutron technique that is truly high resolution on a stand-alone basis.
  - It will be used increasingly to identify key protons in small proteins, nucleic acids and sugars.
- It has already been shown that information obtained at about 1.7Å resolution with neutrons is chemically equivalent to that obtained at 1Å with X-rays.
- Moreover there is no risk of radiation damage which has recently been shown to have a very serious effect on hydrogen atoms in high-resolution X-ray studies.

What are the biological systems amenable to study and which are the techniques most likely to be of use in the Life Sciences?

Small angle scattering – Solution scattering

- will also be a powerful technique at the atomic level by its complementarity with X-ray crystallography.
- cell biology - functioning of very large molecular complexes such as the various molecular motors
  - sub-components of these systems will be isolated and solved to high resolution by X-ray crystallography.
  - to observe conformational changes induced by binding of ions, cofactors etc. Small angle scattering (solution scattering) will allow the docking of known sub-structures at high resolution and a close to in vivo situation and allow easy changes in the solution environment

PAUL SCHERRER INSTITUT

What are the biological systems amenable to study and which are the techniques most likely to be of use in the Life Sciences?

Neutron reflectometry is an emerging technique which has up to now been used most profitably in the field of soft matter chemistry.

- It is however a technique which is perfectly adapted to biological membranes.
- A number of experiments have been carried out largely on reconstituted lipid bilayers or monolayers
  - effort must be put into developing methods of sample preparation for biological systems.
- The development of off-specular scattering to study the in-plane arrangements of membrane proteins is a particularly attractive new development that should be encouraged.

PAUL SCHERRER INSTITUT

What are the biological systems amenable to study and which are the techniques most likely to be of use in the Life Sciences?

Inelastic and quasi-elastic scattering

- have been used with great success to study the dynamics of soft matter.
- They have the great advantage over other spectroscopic techniques that simulated spectra can be exactly calculated and therefore experimental data can be interpreted by, for example, Monte Carlo simulations.
- The range of time scales accessible to neutron scattering is moreover exactly that of interest for the internal dynamics of protein molecules and both amplitude and frequency information are available simultaneously.
- To date the technique has been limited by understanding of the theory and the computing power necessary to carry out appropriate simulations as well as by the large quantities of material (100s of mg) required.
- Technical advances and the availability of materials from modern expression systems should go a long way to improving these problems in the coming years.

Key points for the use of neutrons

The FLUX problem can to some extend be overcome by:

- More material (i.e. where neutrons can provide unique answers)
  - invest in modern techniques (expressions) with higher yield!
  - and with Deuteration capability
- Improved Instrumentation and sources

Outline ----- Nutrons

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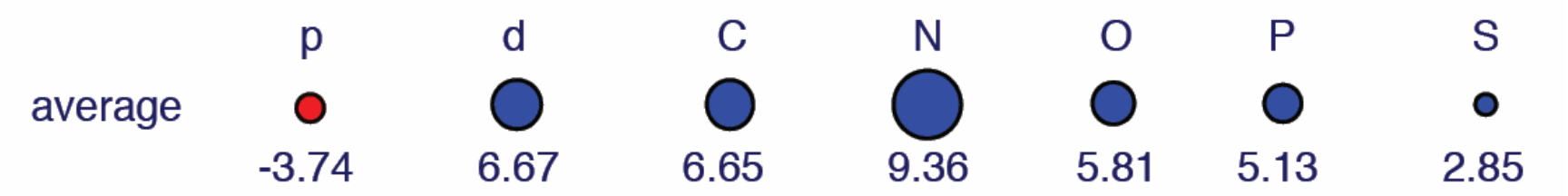
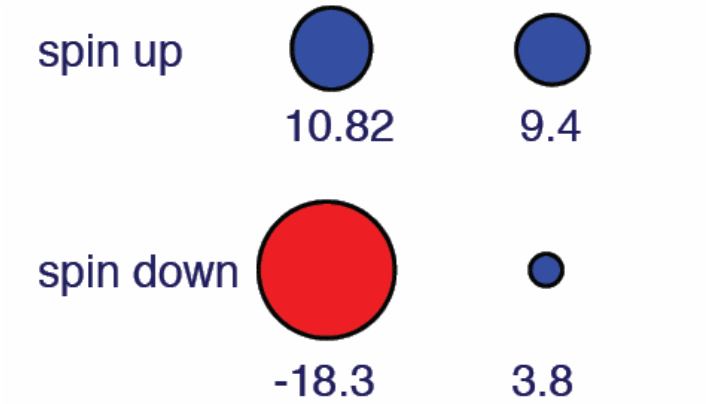
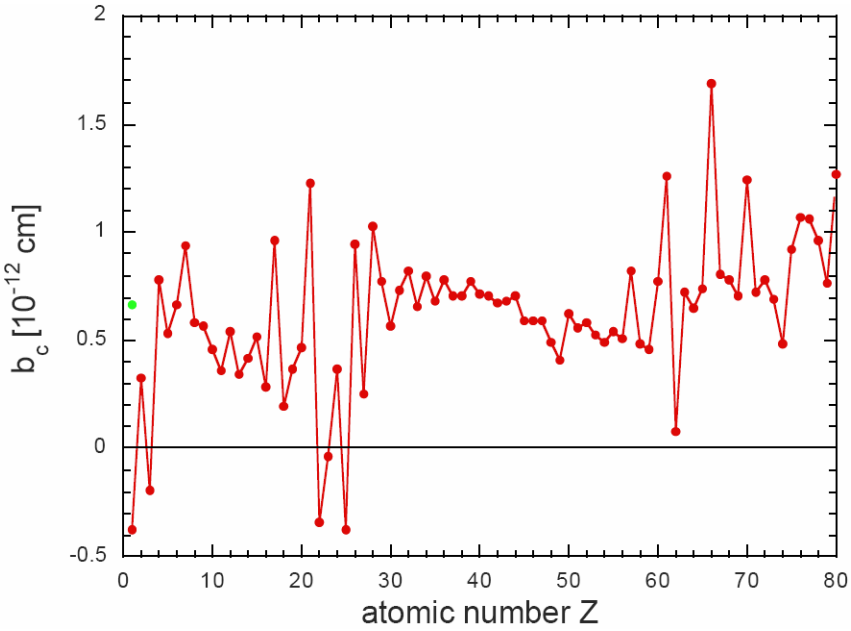
Neutron Scattering Length [fm]





Spin-dependent scattering lengths

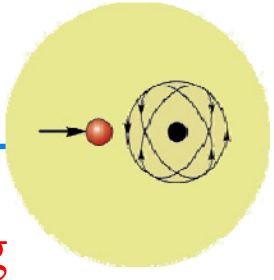


1 fm = 0.1x10^{-12} cm

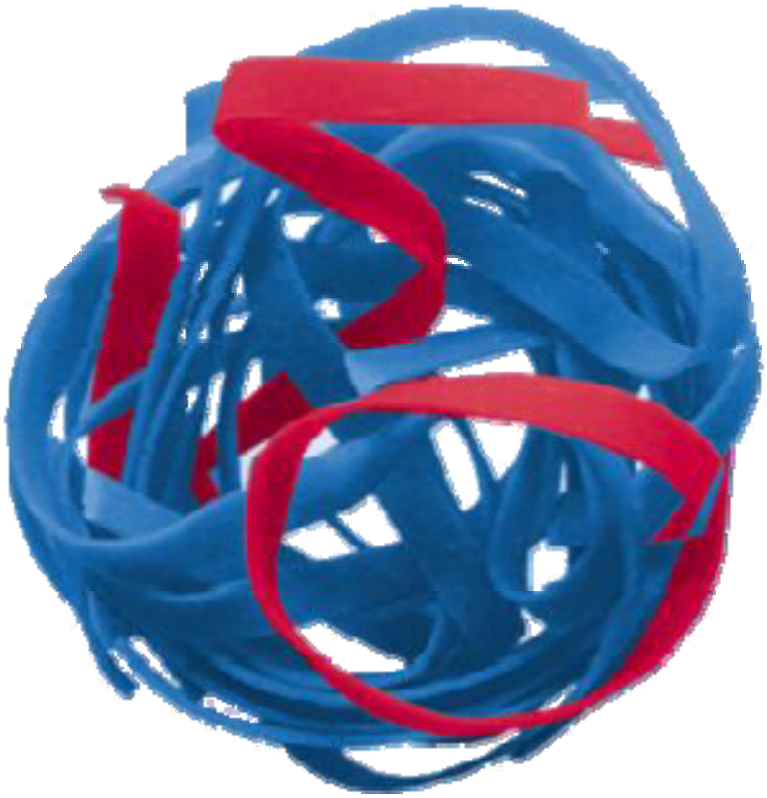
Contrast Variation

J Kohlbrecher PSI

Neutrons see the Nuclei



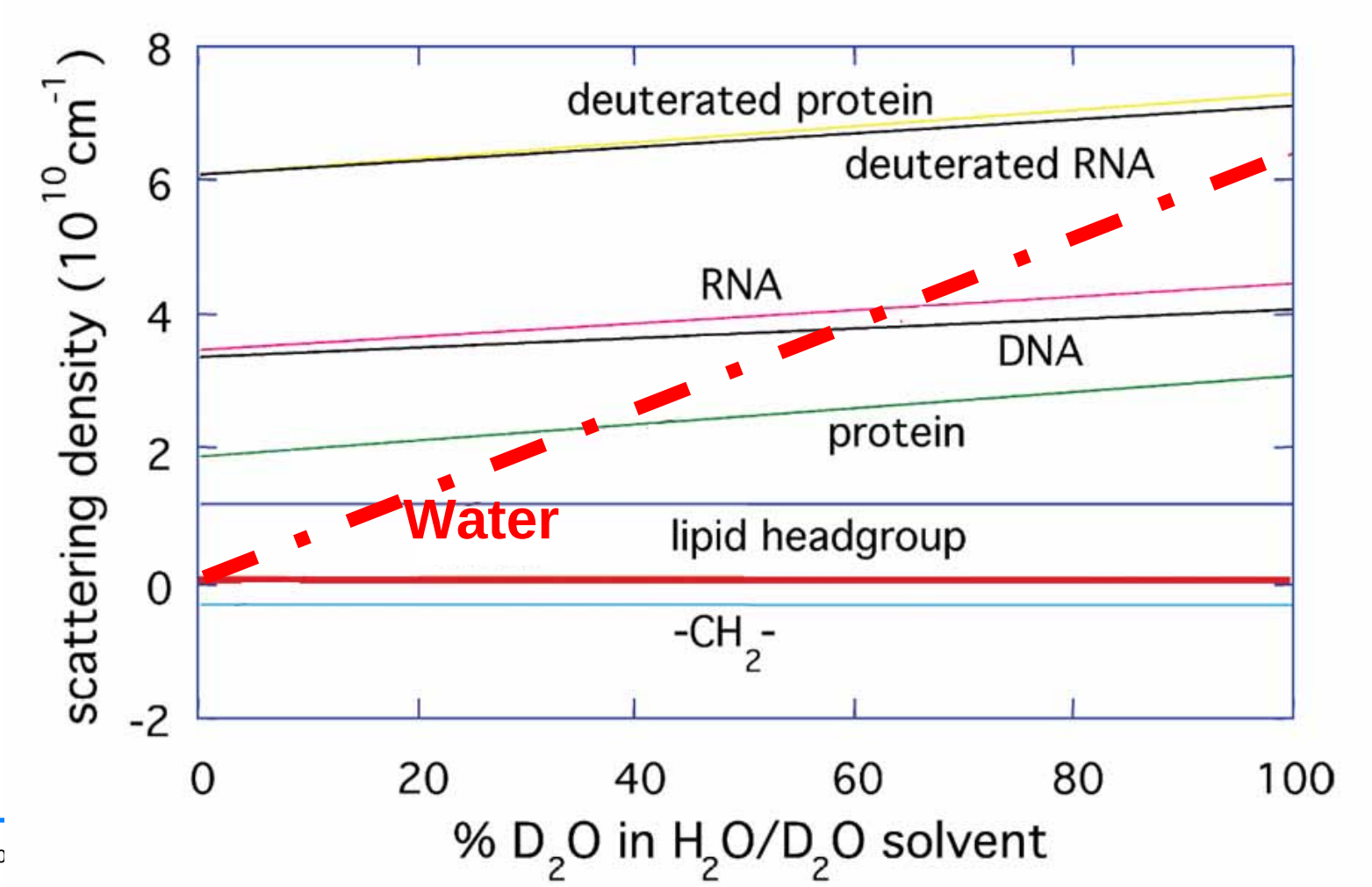
Follow polymer dynamics with spin echo neutron scattering



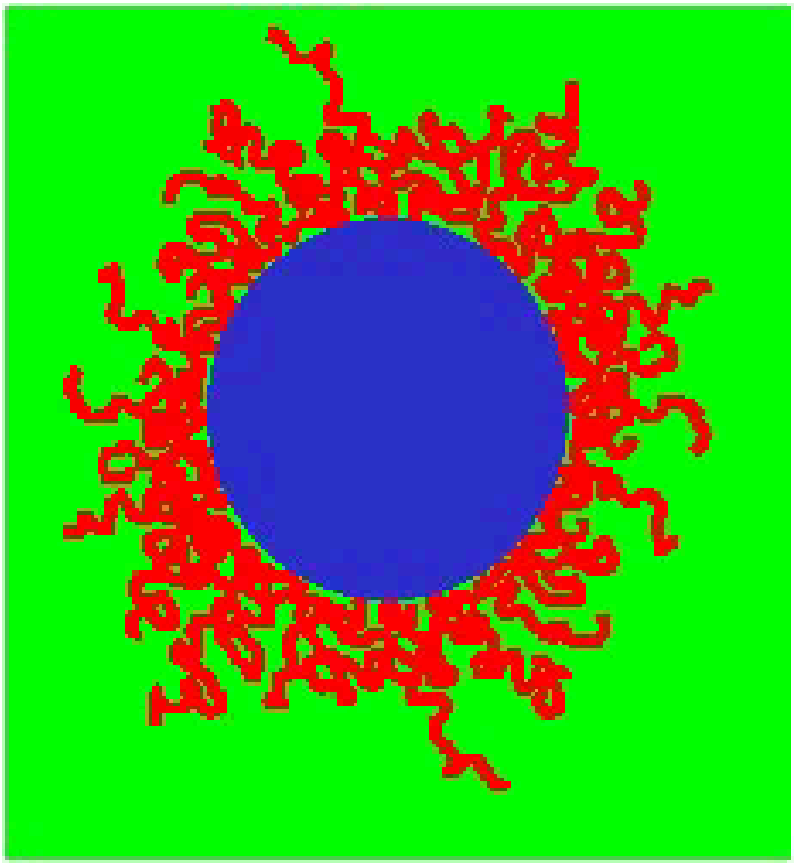
See presentation by M Monkenbush 24-25/11

Contrast Variation

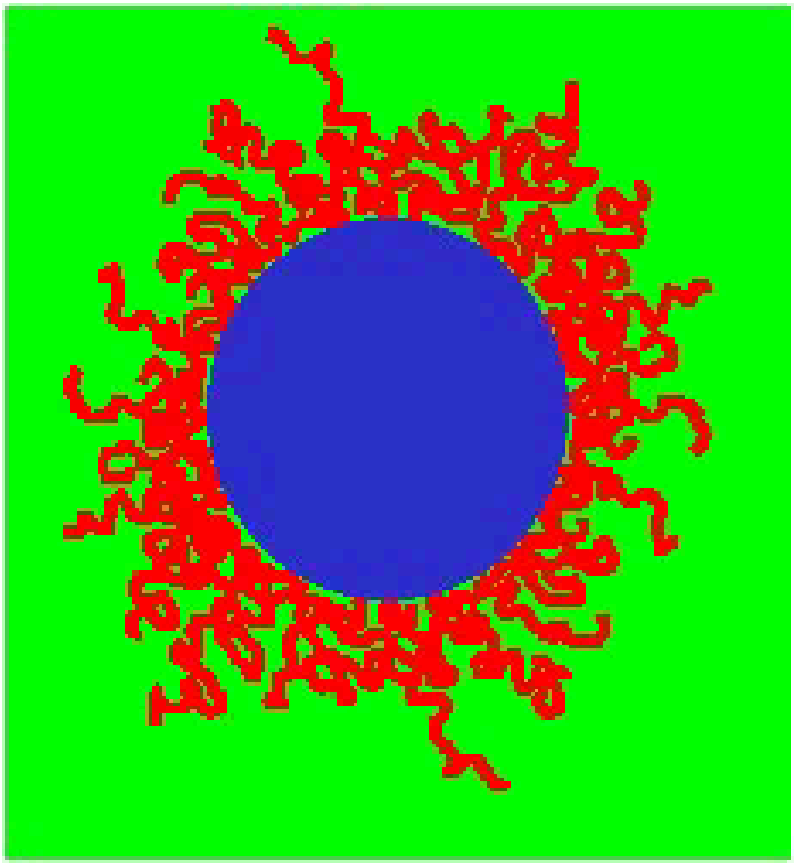
- A different fraction of hydrogen leads to a different scattering length density
- Solvent contrast variation: H_2O/D_2O mixtures match different material at different D_2O percentage



Contrast Variation



matching of core



matching of shell

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Small Angle Neutron Scattering

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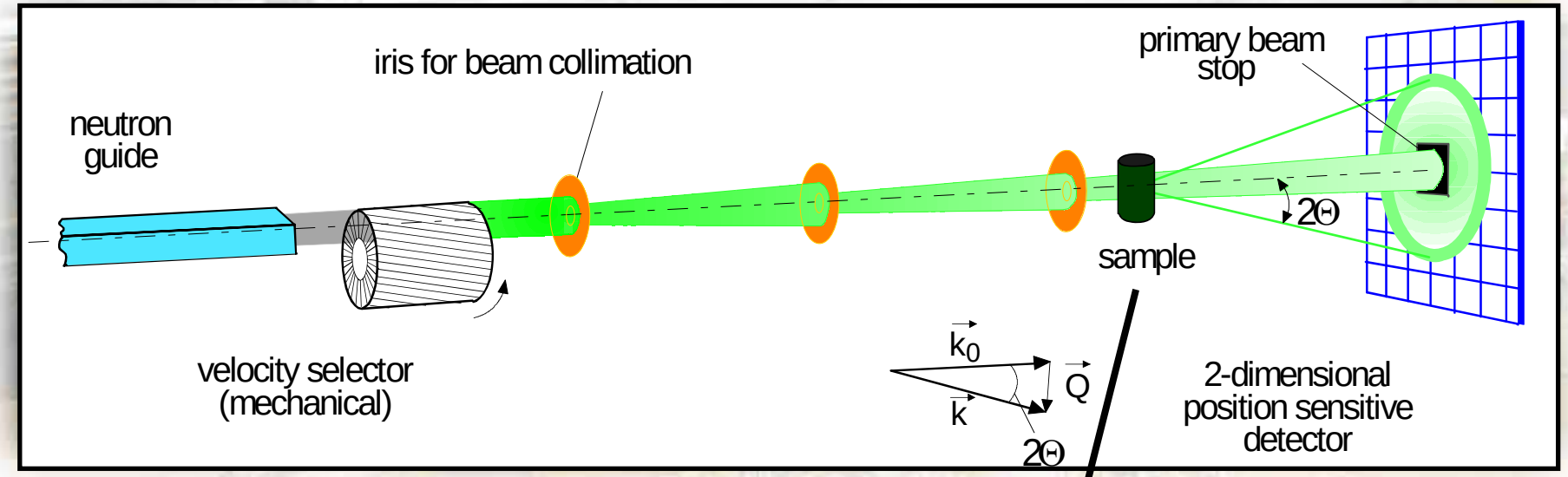
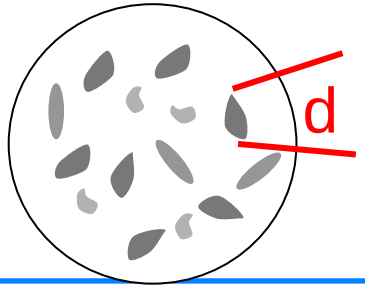


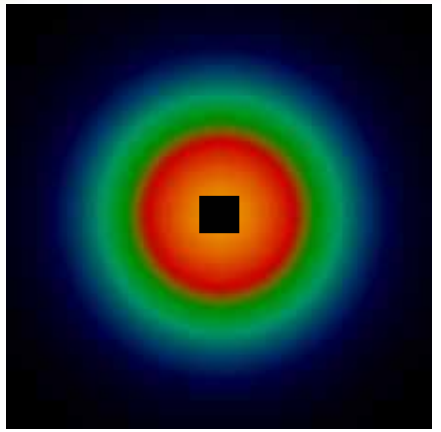
$$\frac{2\pi}{d} = Q = \frac{4\pi}{\lambda}\sin\left(\theta/2\right)$$

$\lambda \approx 0.5$ nm

d $\approx$ 10 nm

$\Rightarrow \theta \approx 3$ deg

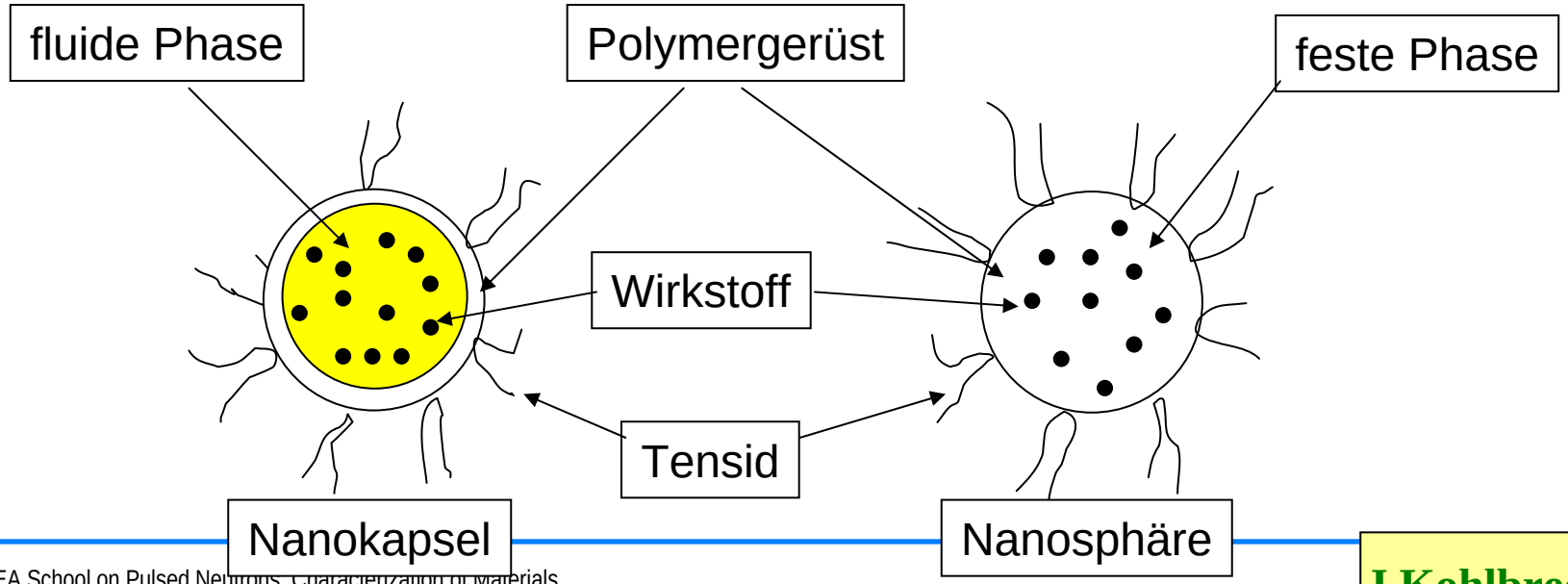




Drug Targeting: Core-Shell Structure of Poly(D,L-lactide) Nanocapsules

Andrea Rübe[1], Gerd Hause[2], Karsten Mäder[1], Joachim Kohlbrecher[3*]
[1]Institute of Pharmaceutical Technology and Biopharmacy, Martin-Luther-University Halle-Wittenberg
[2]Microscopy Unit, Biocenter of the University, Halle/Saale
[3]Laboratory for Neutron Scattering, Paul Scherrer Institute

- **Einschluss von lipophilen Wirkstoffen in die innere Ölphase möglich**
- **Tensidschicht umgibt Nanokapseln, um sie im Wasser zu stabilisieren**



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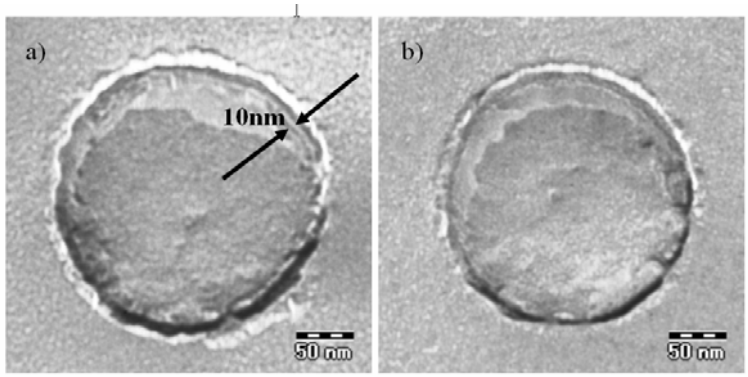

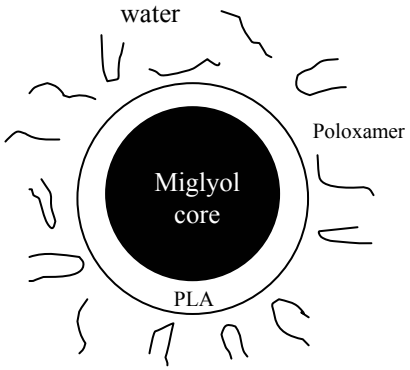

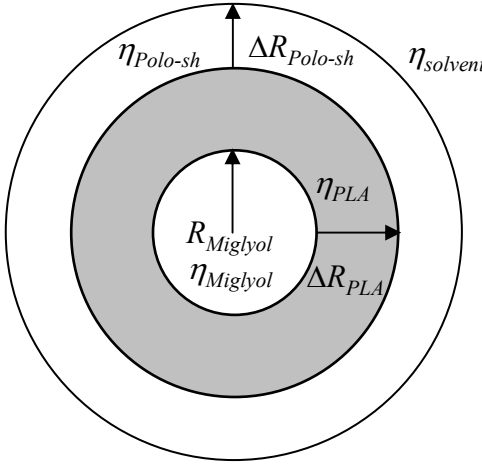

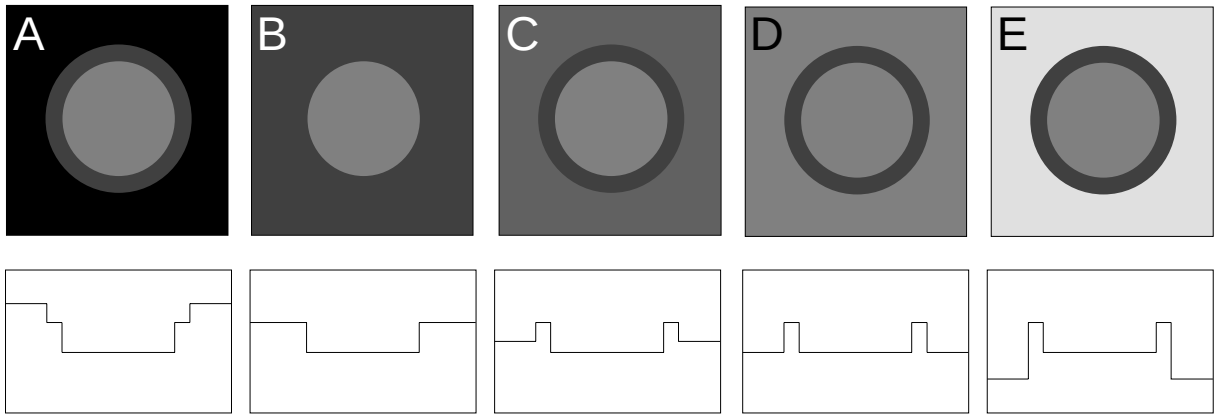

A→D different H20/D2O mixture in solvent

Andrea Rübe[1], Gerd Hause[2], Karsten Mäder[1], Joachim Kohlbrecher[3*]

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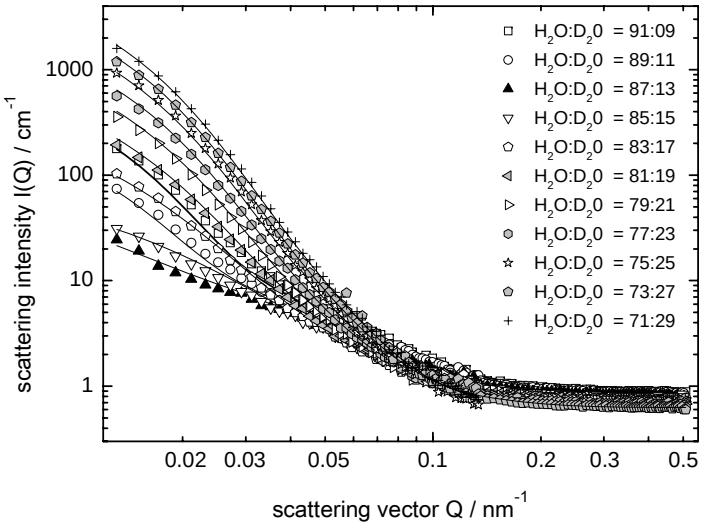
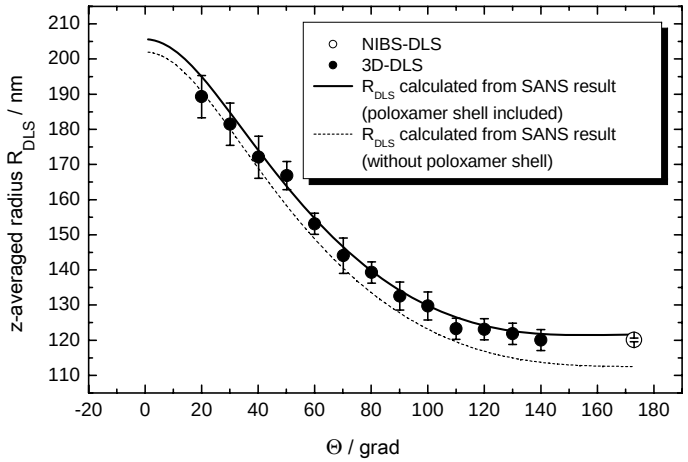
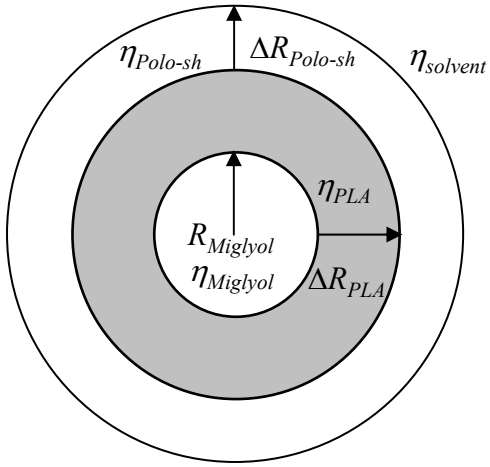
Drug Targeting: Core-Shell Structure of Poly(D,L-lactide) Nanocapsules







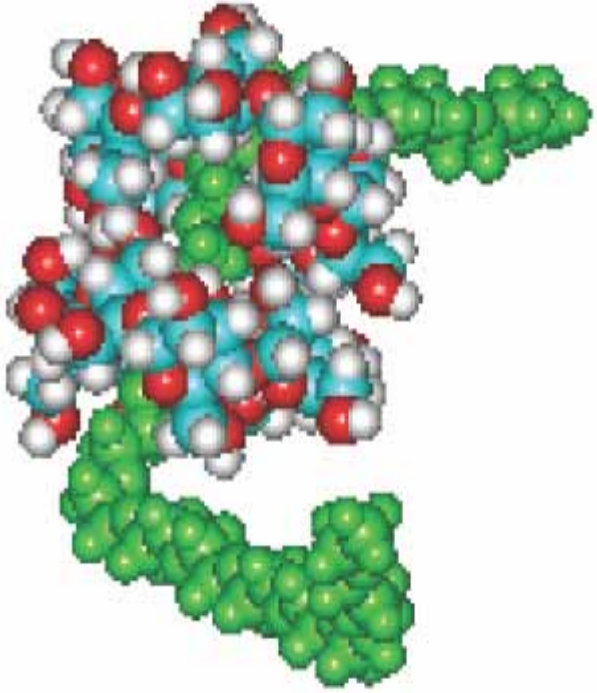
σ = 0.394,
R_0 = 84 nm,
ΔR_{PLA} = 9.8 nm
$\Delta R_{Polo\text{-}sh}$=17 nm
Poloxamer concentration in outer shell of 7%.

J Kohlbrecher PSI

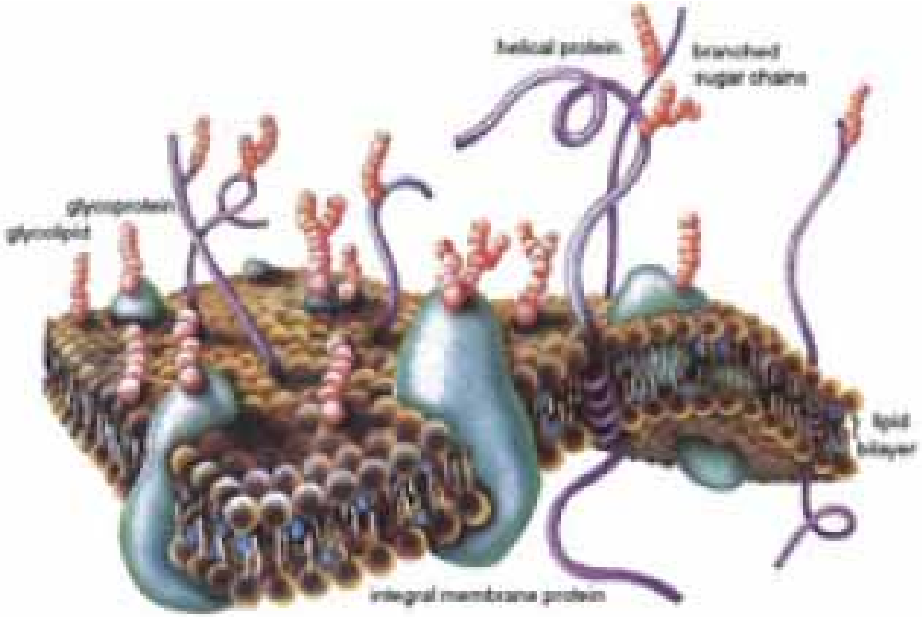
From solutions → Membranes

Atomic resolution structures of the different constituent molecules in general from Synchrotron X-ray diffraction

Relative orientation of components from solution scattering

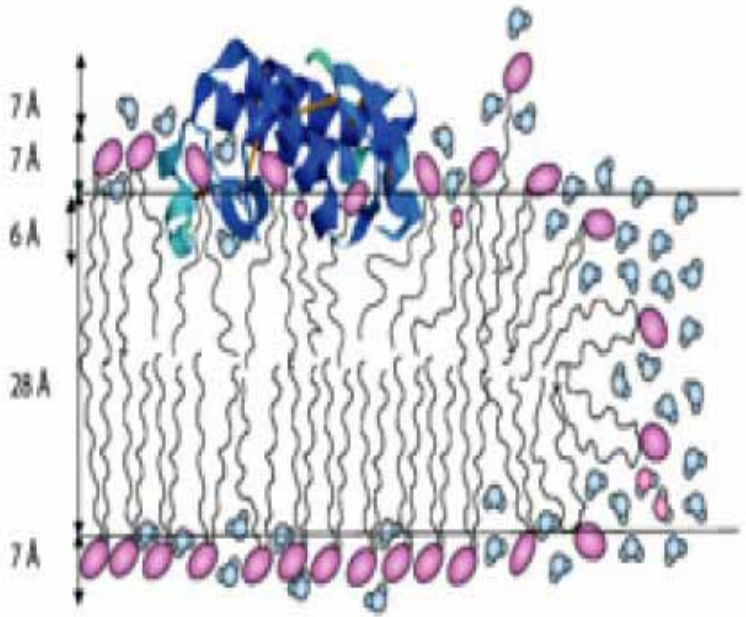


Self assembled polyrotaxanes (polymer complexes)



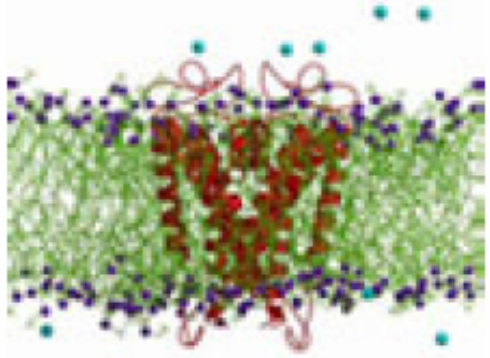
The cell membrane, showing the location of proteins and other cellular material within the phospholipid bilayer

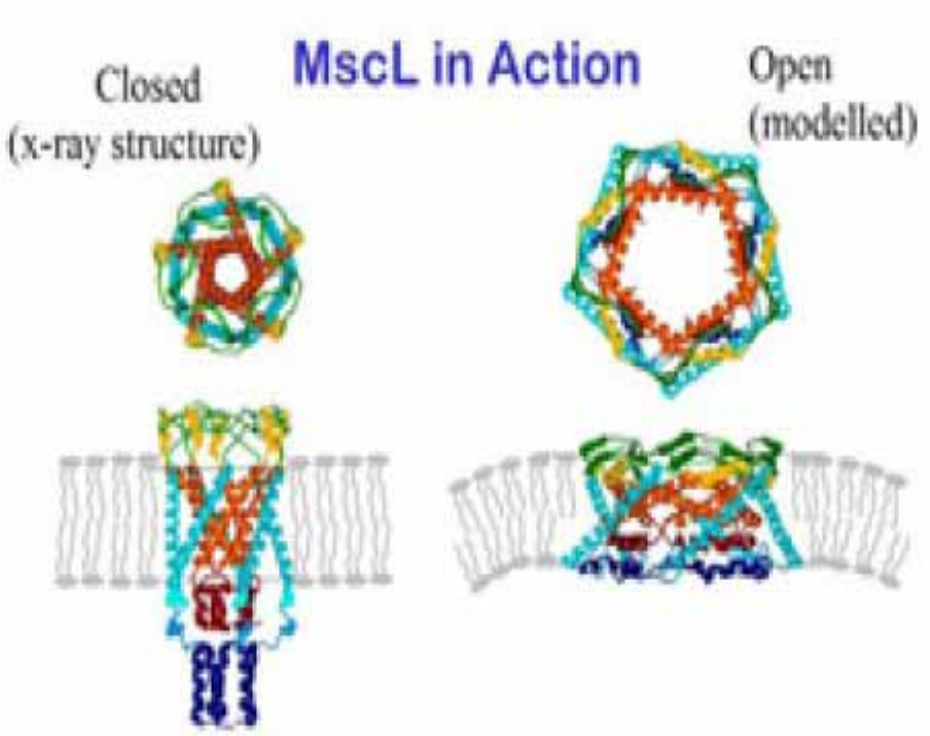
Function .....



Schematic representation of Phospholipase A2 interacting with a phospholipid bilayer, derived from neutron reflectometry.

Natural Antibiotics



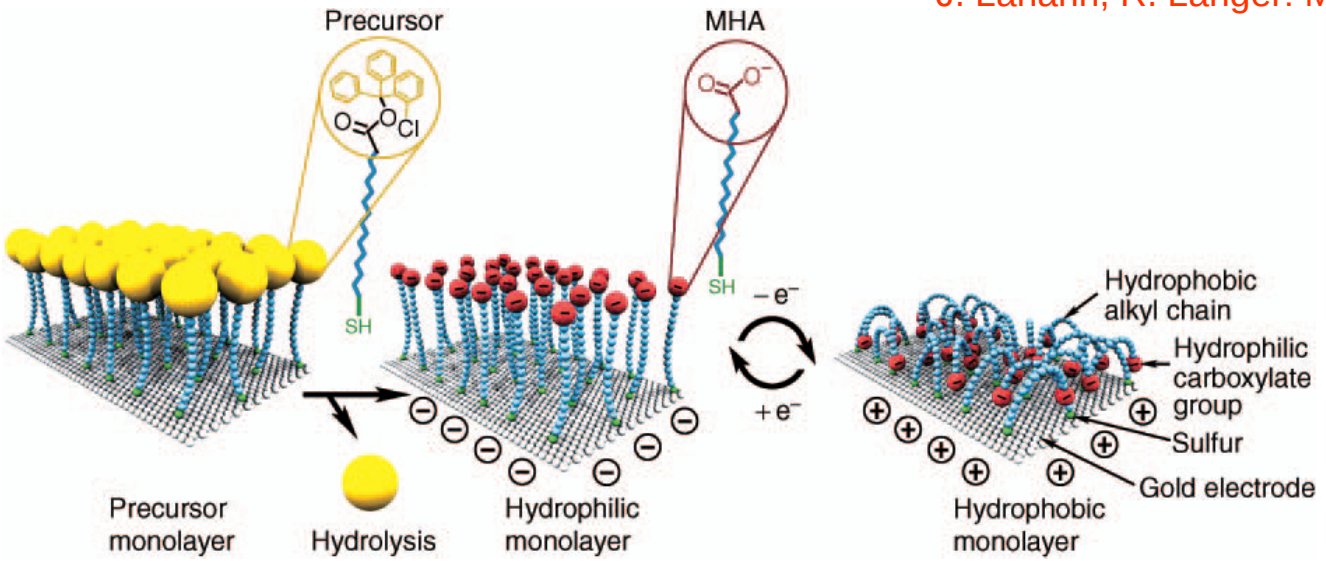


Schematic representation of the proposed mechanism of the MscL channel.

Biomimetics – functional surfaces

Dynamically Controlled Surface Properties (T, pH, Light, V, etc.)

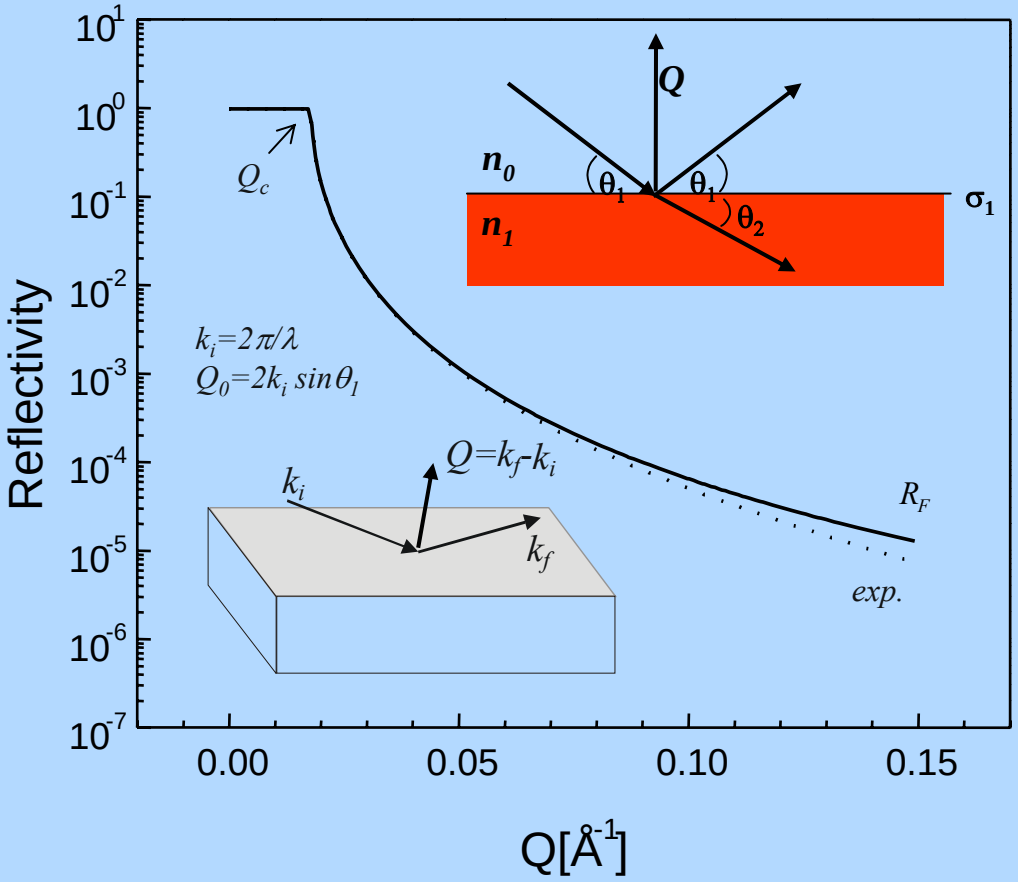
J. Lahann, R. Langer: MRS Bulletin



Applications:

- Biosensors
- Microfluidic devices (valves, reservoirs)
- Structural templates for tissue engineering
- Drug delivery
- Study of cell/cell and cell/protein interactions

Biomembranes and Interfaces



Reflectivity of a single interface (Fresnel reflectivity)

$$R = r\,r^*$$

$$r = A'_1/A_1 = (Q_0-Q_1)/(Q_0+Q_1)$$ reflection coefficient

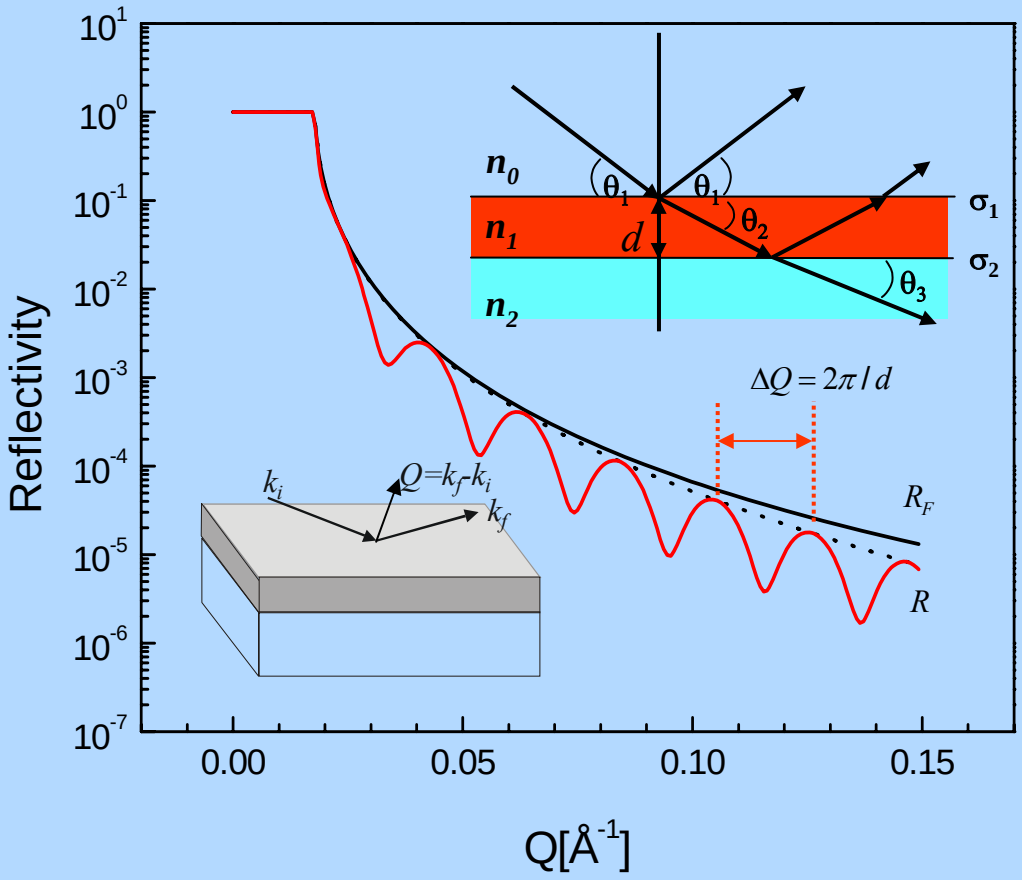
with $Q_i = (Q_0^2-Q_c^2)^{1/2}$

$$R_F(Q) = \left|\frac{1-[1-(Q_c/Q_0)^2]^{1/2}}{1+[1-(Q_c/Q_0)^2]^{1/2}}\right|^2$$

for $Q_0 > Q_c$

$$R_F(Q) \approx (Q_c/Q_0)^4$$

Biomembranes and Interfaces



Reflectivity of two interfaces

$$R(Q) = \frac{r_1^2 + r_2^2 + 2r_1 r_2 \cos(2Q_1 d)}{1 + r_1^2 r_2^2 + 2r_1 r_2 \cos(2Q_1 d)}$$

with thickness $d = 2\pi/\Delta Q$

in kinematic theory

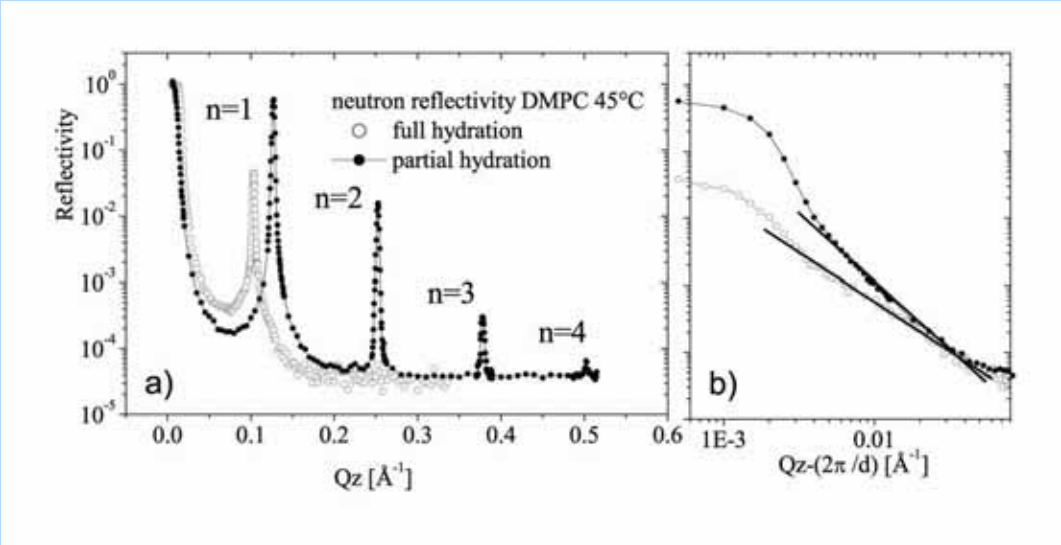
$$r = \frac{(k_c^2)^2}{Q_0^4} \left| \int \frac{d\rho}{dz} \cdot \exp(iQ_0 z) dz \right|^2$$

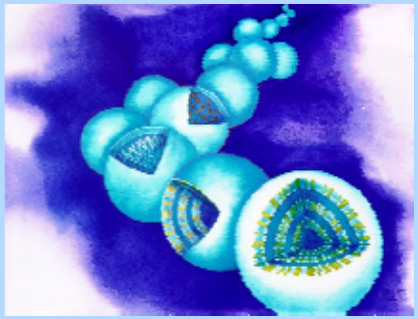
reflectivity of two interfaces

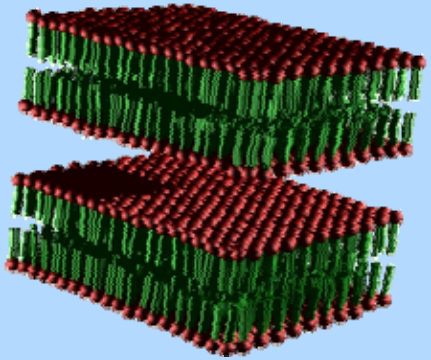
$$R(Q) = \frac{(k_c^2)^2}{Q^4} \left[\begin{array}{l} \Delta\rho_1 \cdot \exp\left(-Q^2\sigma_1^2\right) + \Delta\rho_2 \cdot \exp\left(-Q^2\sigma_2^2\right) \\ + \Delta\rho_3 \cdot \exp\left(-Q^2\left(\sigma_1^2 + \sigma_2^2\right)/2\right) \cdot \cos(Q\mathrm{d}) \end{array} \right]$$

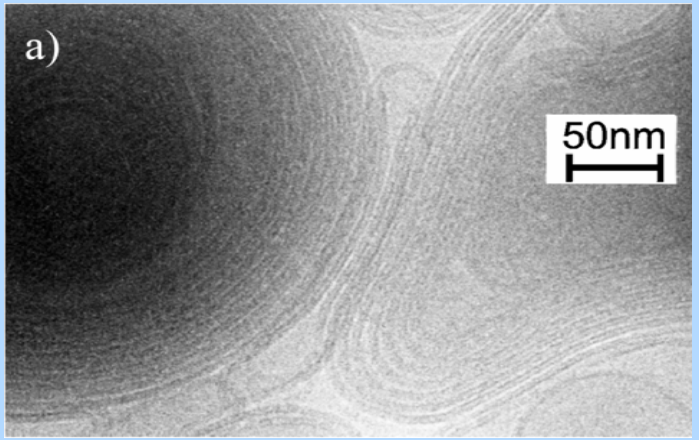
with parameters d, σ, $\Delta\rho$

Biomembranes





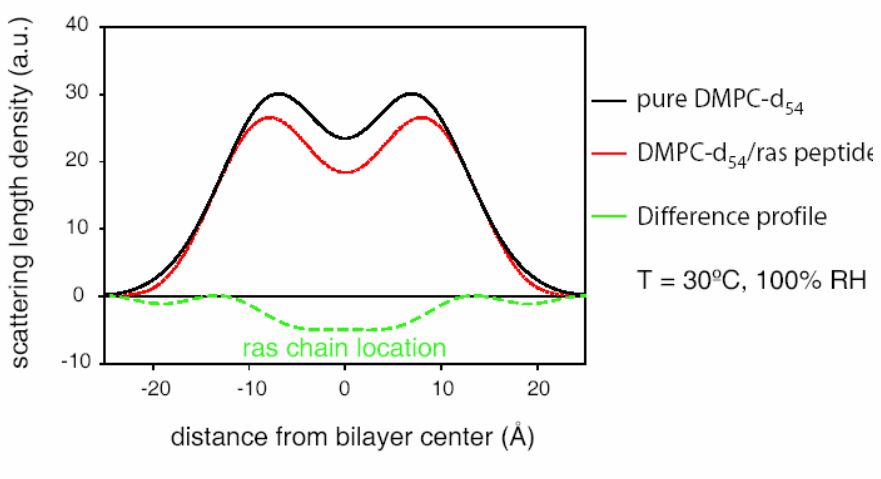


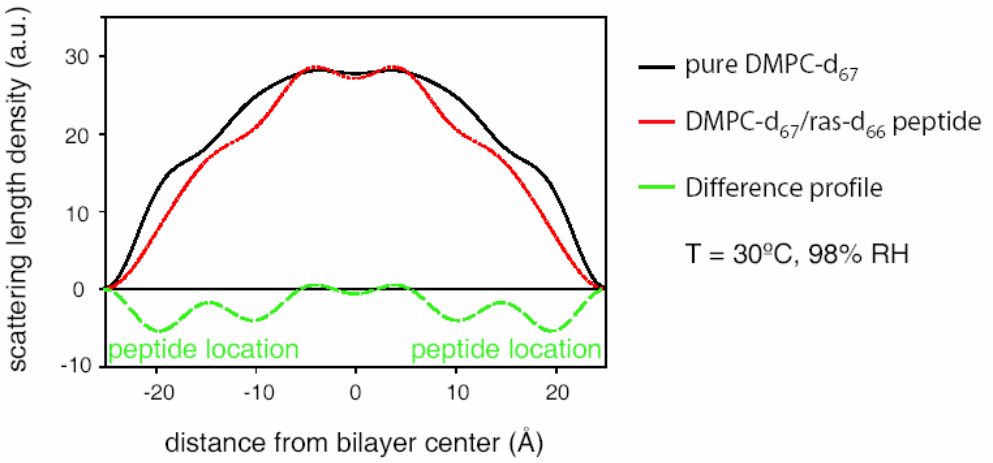


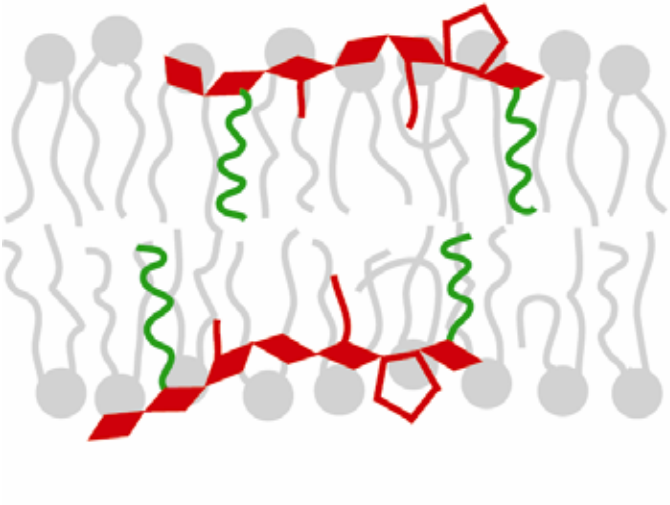
multilamellar vesicles

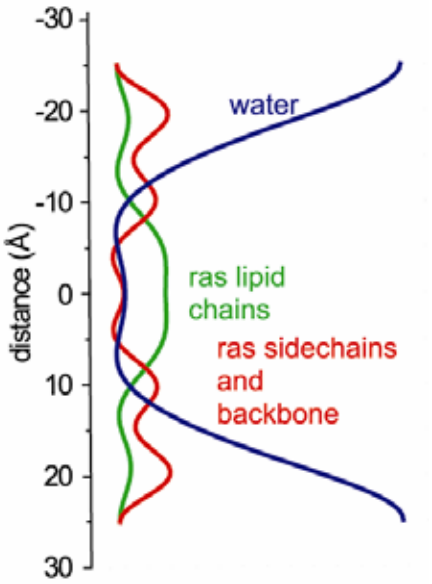
(from B. Klösgen in Lipid Bilayers - Structure and Interactions)

Membrane Binding of Lipidated N-ras Peptide









T Gutberlet PSI

(D. Huster et al., JACS, 125, 2003, 4070)

Biomembranes and Interfaces

Anchoring of Recombinant Proteins to Functionalized Phospholipid Monolayers

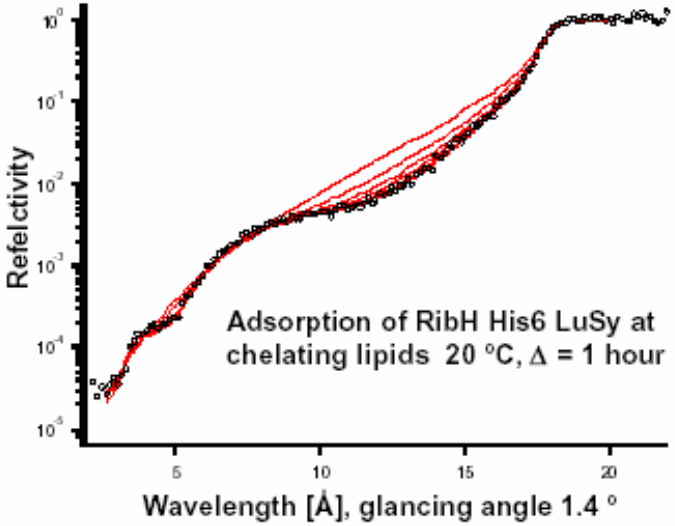


Figure 1. Reflectivity data obtained during the adsorption of LuSy to a Ni Chelator covered surface. The lines correspond to the best fits of the neutron reflectivity data sets, plotted over wavelength. The time distance between two sets of data is one hour.

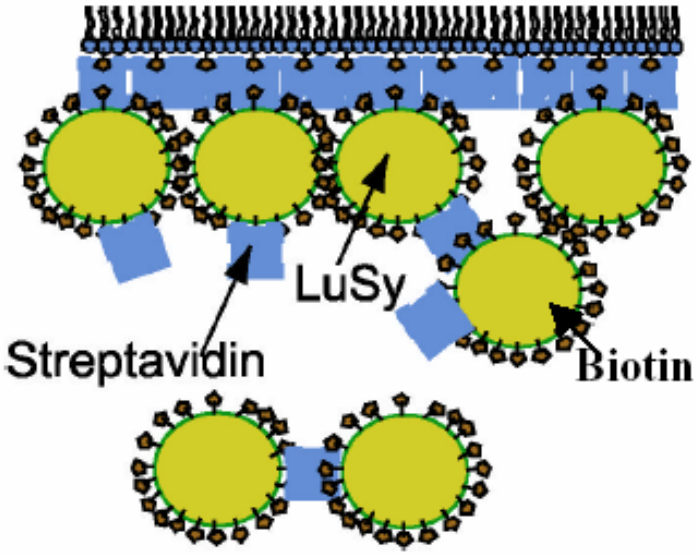
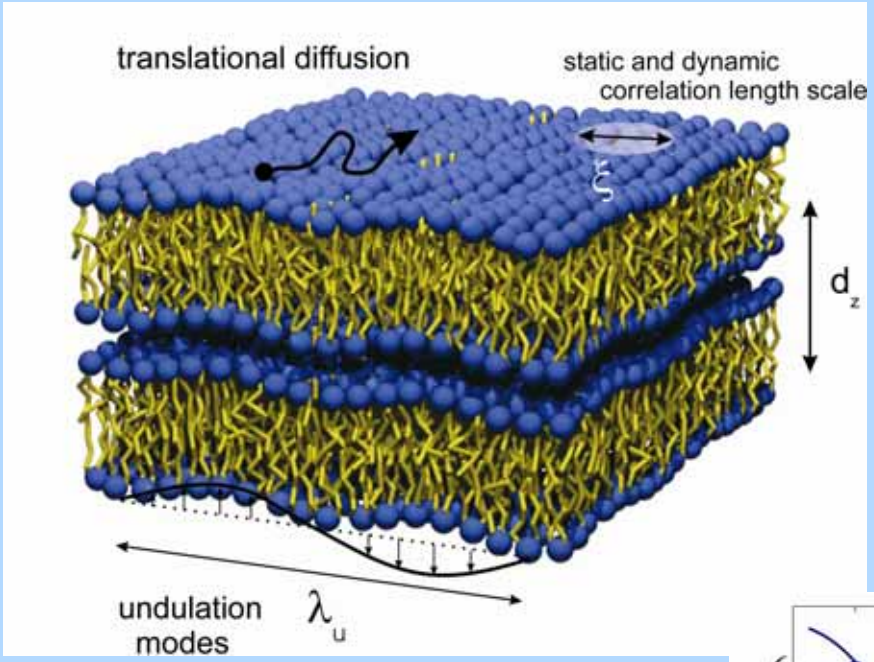


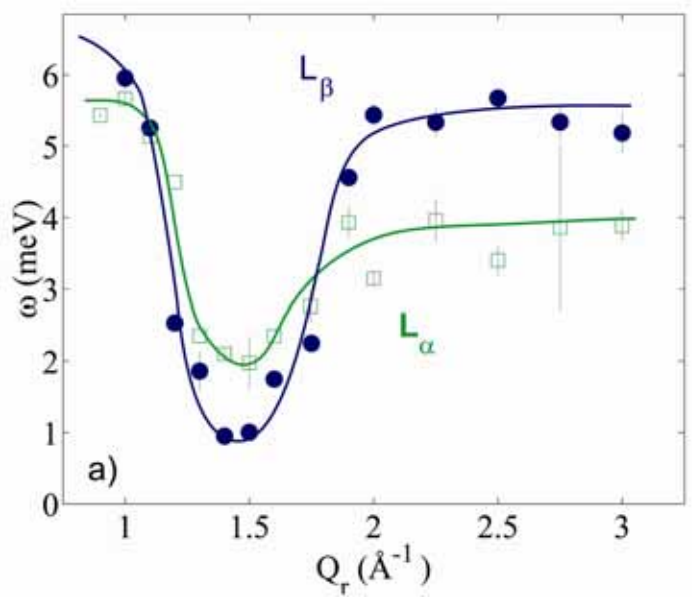
Figure 4. Model of multilayers to fit the data of biotin Lusy adsorbed to a streptavidin interface

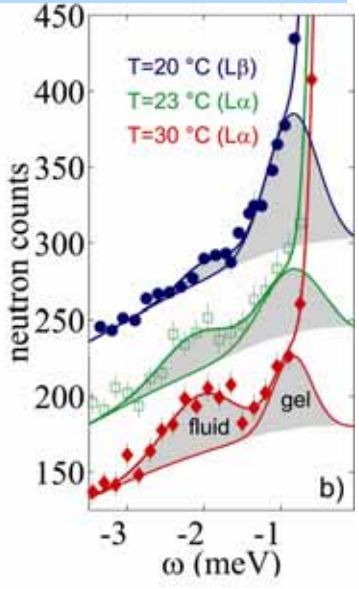
M. Tristl et al., LLB Scientific Report 1999-2000, 100

Biomembranes - dynamics

T Gutberlet PSI



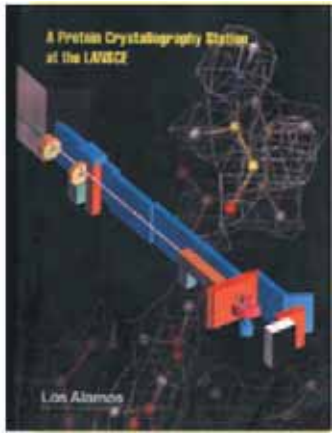


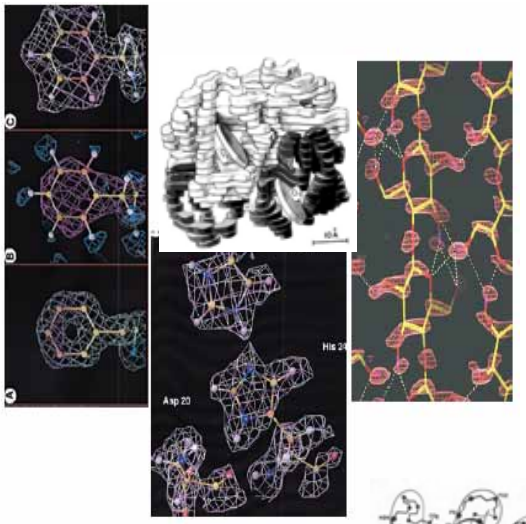


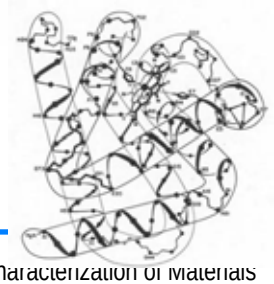
PCS Station LANCSE

Paul Langan / Benno Schoenborn

J Schefer, PSI







Example above:

Myoglobin, 17kD, 35 A, hydrogen shell

PCS Specifications

Protein crystallography – an existing facility!

Unit cell size 150 Å

d-spacing 1 Å - 250 Å

Wavelength shapingT0 and T1 choppers and tail-cutter

Wavelength range 1-5 Å

Sample-to-detector distance 700 mm

Beam size 5 mm on detector

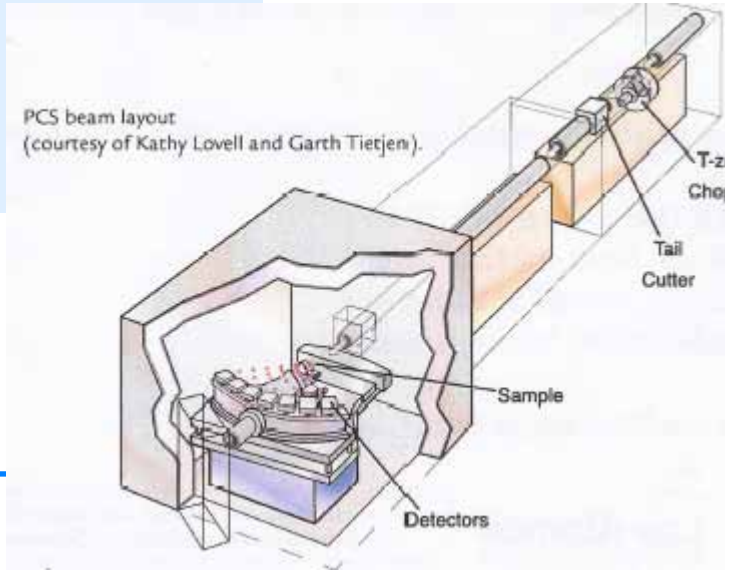
Detector resolution 1.2 mm

Detector area 120°, R=70cm, H=20cm

Counting rate> 1,000,000 c/s

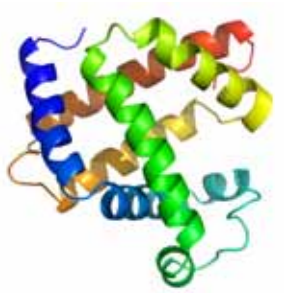
7 10^6 $ncm^{-2}s^{-1}$ at 100 µA (1-5Å)

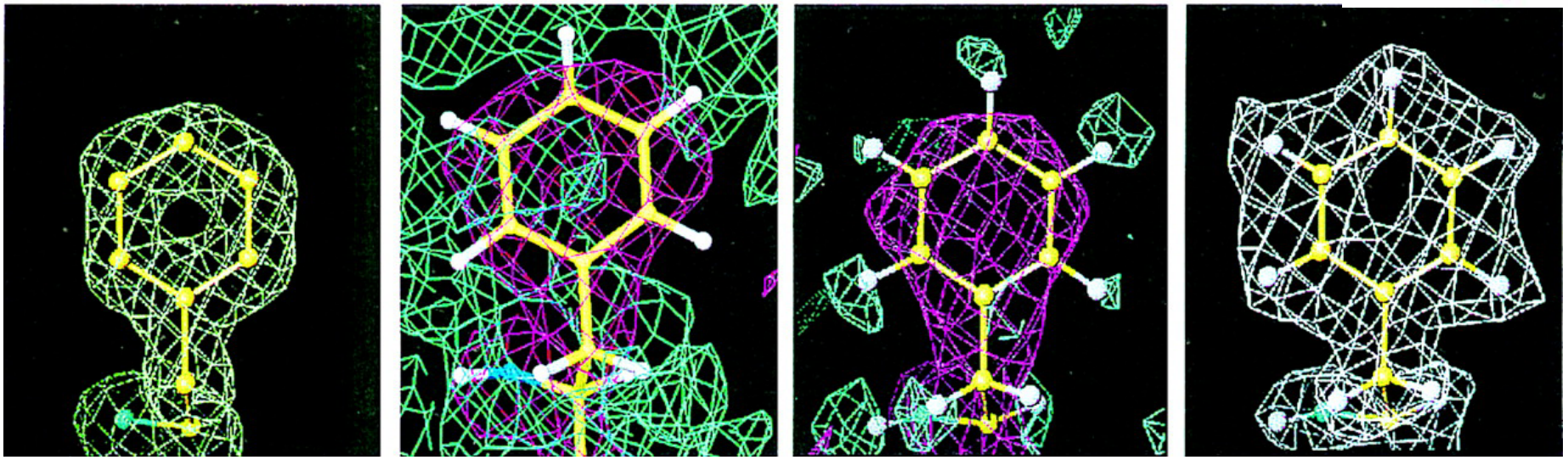
1-10 days/protein



High Resolution Neutron Crystallography

(example: hydrogen in Myoglobin, 17 kD)





X-Ray

neutrons
unlabelled

Calculated
from (B)

neutrons
Fully deuterated

Neutrons:
Location of hydrogen from from low resolution data (~2Å) possible,
Even if paramagnetic metal ions are in the vicinitiy (kills NMR)

Shu et al, Proceedings of the National Academy of Science, **97**(8), 3872-3877 (2000)

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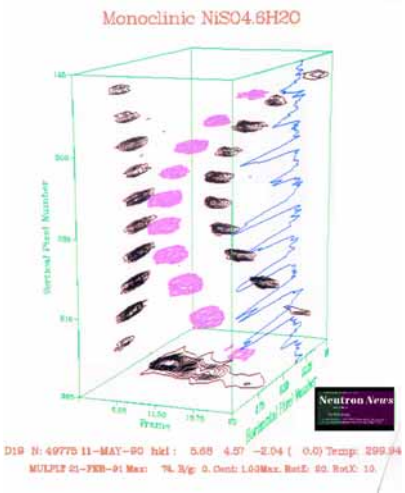
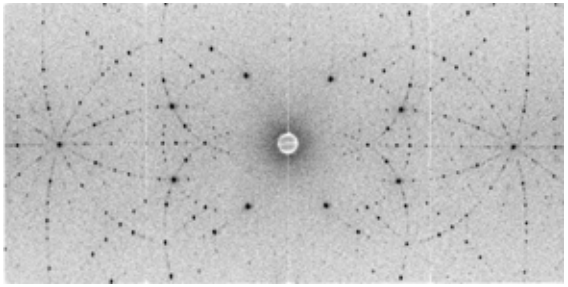
Present

Future



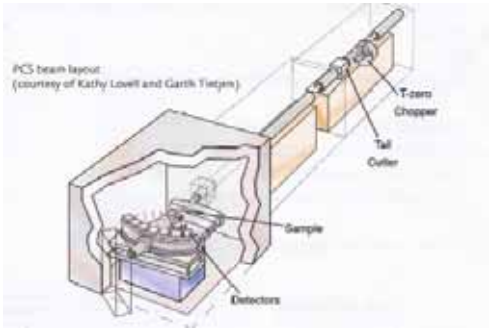
D19 / ILL



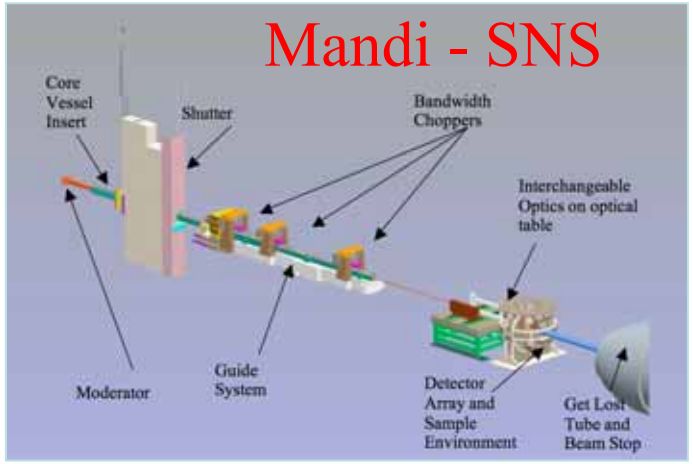
LADI / ILL
(V<300'000 Å³)

J-Parc
Japan

Bio–Molecule Diff. (Ibaraki Pref.)

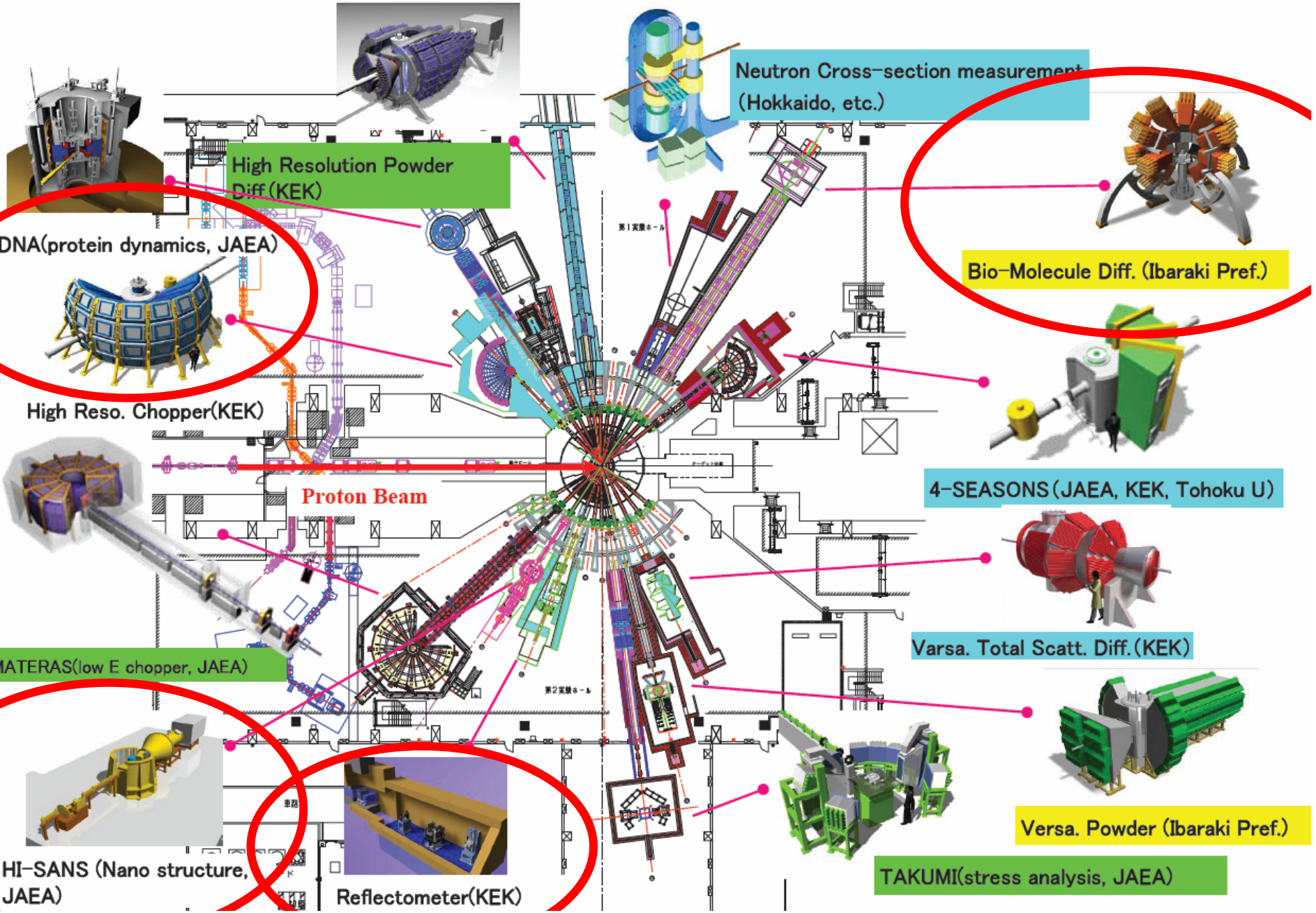


PCS / LANSCE

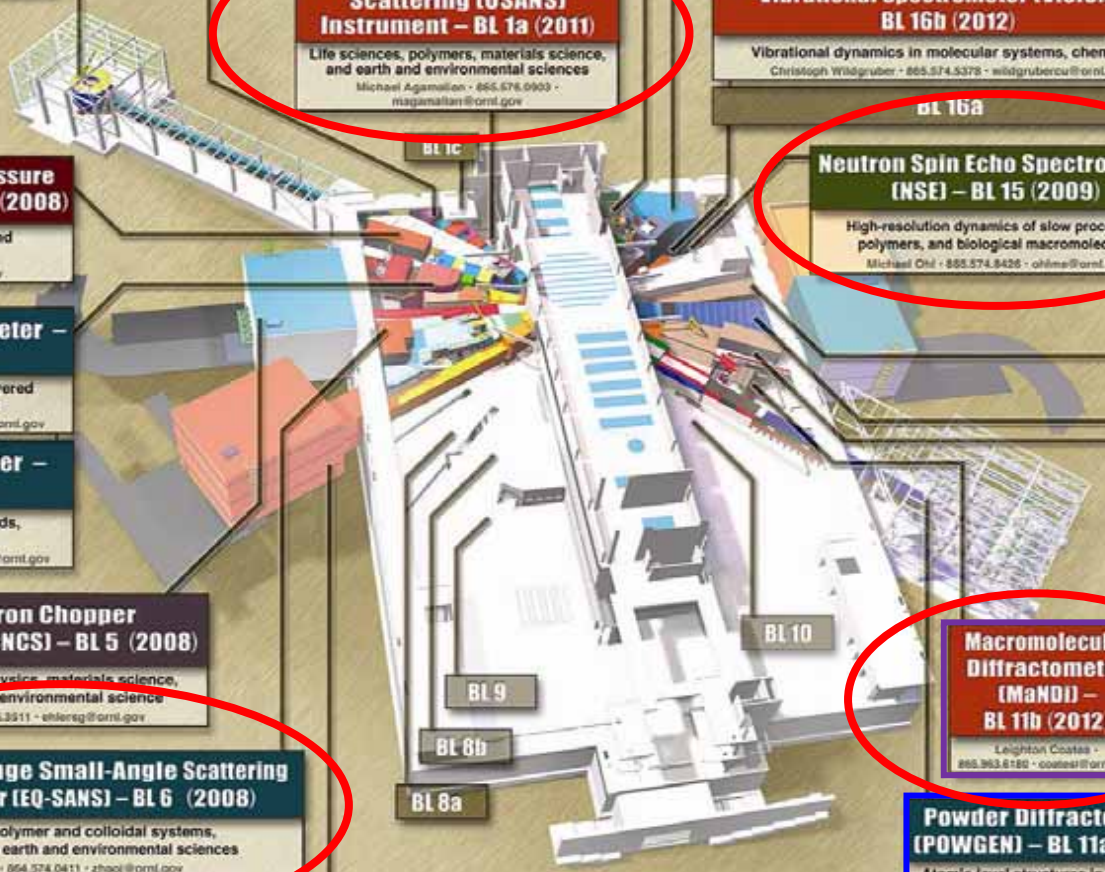


Neutron Instruments under construction (color labeled) and planned

JAEA or KEK、 Ibaraki Pref. Grant



Spallation Neutron Source



Backscattering Spectrometer (BASIS) – BL 2 (2006*)
Dynamics of macromolecules, constrained molecular systems, polymers, biology, chemistry, materials science

Nanoscale-Ordered Materials Diffractometer (NOMAD) – BL 1b (2010)
Liquids, solutions, glasses, polymers, nanocrystalline and partially ordered complex materials
Joerg Neuefeind · 865.241.1635 · neuefeindjc@ornl.gov

Wide Angular-Range Chopper Spectrometer (ARCS) – BL 18 (2007)
Atomic-level dynamics in materials science, chemistry, condensed matter sciences
Doug Abernathy · 865.576.5109 · abernathydl@ornl.gov

Fine-Resolution Fermi Chopper Spectrometer (SEQUOIA) – BL 17 (2008)
Dynamics of complex fluids, quantum fluids, magnetism, condensed matter, materials science
Garrett Granroth · 865.576.0900 · granrothge@ornl.gov

Ultrasmall-Angle Neutron Scattering (USANS) Instrument – BL 1a (2011)
Life sciences, polymers, materials science, and earth and environmental sciences
Michael Agamalian · 865.576.0903 · magamalian@ornl.gov

Vibrational Spectrometer (VISION) – BL 16b (2012)
Vibrational dynamics in molecular systems, chemistry
Christoph Wildgruber · 865.574.5378 · wildgrubercu@ornl.gov

BL 16a

BL 1c

Neutron Spin Echo Spectrometer (NSE) – BL 15 (2009)
High-resolution dynamics of slow processes, polymers, and biological macromolecules
Michael Ohl · 865.574.8426 · ohlme@ornl.gov

Hybrid Chopper Spectrometer (HYSPEC) – BL 14B (2011)
Atomic-level dynamics in single crystals, magnetism, condensed matter sciences
Mark Hagen · 865.241.9782 · hagenmr@ornl.gov

BL 14a

Spallation Neutrons and Pressure Diffractometer (SNAP) – BL 3 (2008)
Materials science, geology, earth and environmental sciences
Chris Tulk · 865.576.7038 · tulkca@ornl.gov

Magnetism Reflectometer – BL 4a (2006)
Chemistry, magnetism of layered systems and interfaces
Frank Klose · 865.576.5389 · kloseb@ornl.gov

Liquids Reflectometer – BL 4b (2006)
Interfaces in complex fluids, polymers, chemistry
John Ankner · 865.576.5122 · ankneri@ornl.gov

Fundamental Physics Beam Line – BL 13 (2008)
Fundamental properties of neutrons
Geoffrey Greene · 865.574.8435 · greenegl@ornl.gov

Single-Crystal Diffractometer (TOPAZ) – BL 12 (2009)
Atomic-level structures in chemistry, biology, earth science, materials science, condensed matter physics
Christina Hoffmann · 865.576.5127 · hoffmannch@ornl.gov

Cold Neutron Chopper Spectrometer (CNCS) – BL 5 (2008)
Condensed matter physics, materials science, chemistry, biology, environmental science
Georg Ehlers · 865.576.3911 · ehlersg@ornl.gov

BL 10

BL 9

BL 8b

BL 8a

Macromolecular Diffractometer (MaNDi) – BL 11b (2012)
Leighton Coates · 865.963.6180 · coatesl@ornl.gov

Extended Q-Range Small-Angle Scattering Diffractometer (EQ-SANS) – BL 6 (2008)
Life science, polymer and colloidal systems, materials science, earth and environmental sciences
Jinkui Zhao · 864.574.0411 · zhaoj@ornl.gov

Powder Diffractometer (POWGEN) – BL 11a (2008)
Atomic-level structures in magnetism, chemistry, materials sciences
Jason Hodges · 865.576.7034 · hodgesj@ornl.gov

Engineering Materials Diffractometer (VULCAN) – BL 7 (2008)
Engineering, materials science, materials processing
Xun-Li Wang · 865.574.9164 · wangxl@ornl.gov

* Date shown is the scheduled commissioning date.

LEGEND

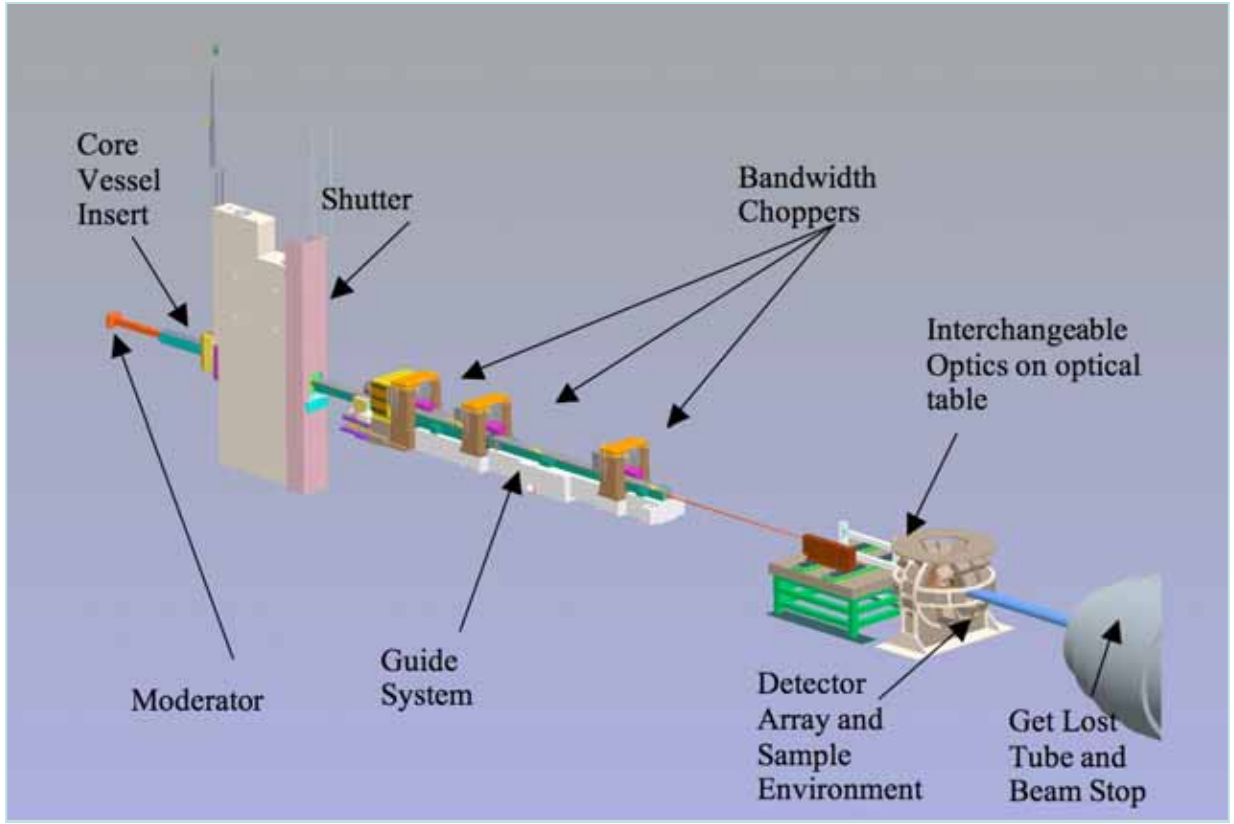
SNS TPC	SING 1	SING 2
DOE Grant	DOE NP	Non U.S.

OAK RIDGE National Laboratory

NEUTRON SCIENCES

06-G00400E/arm

MaNDI - Macromolecular Diffractometer



- **Large solid angle detector coverage**
- **Crystal sizes: ~0.1mm^3 and below**
- **Reduced data collection time (1 day to 1 Week)**
- **Resolution 1.5-2.0 Å (D_{min})**
- **Large unit cell repeats 150-300 Å**

Nanomaterials, Structural Biology and Enzmology

I Anderson, SNS

Protein Unfolding in Presence of Surfactant

PSI-BARC Collaboration
J. Kohlbrecher, R. Vavrin (LNS-PSI, Switzerland)
V.K. Aswal (BARC, Mumbai, India)

mixture of protein and surfactant complexes:

used in a variety **pharmaceutical**, **cosmetic** and **food** products

both share the property of charged groups and hydrophobic portions

Do surfactant molecules undergo electrostatic binding to the protein?
Can surfactant molecules denaturate proteins?

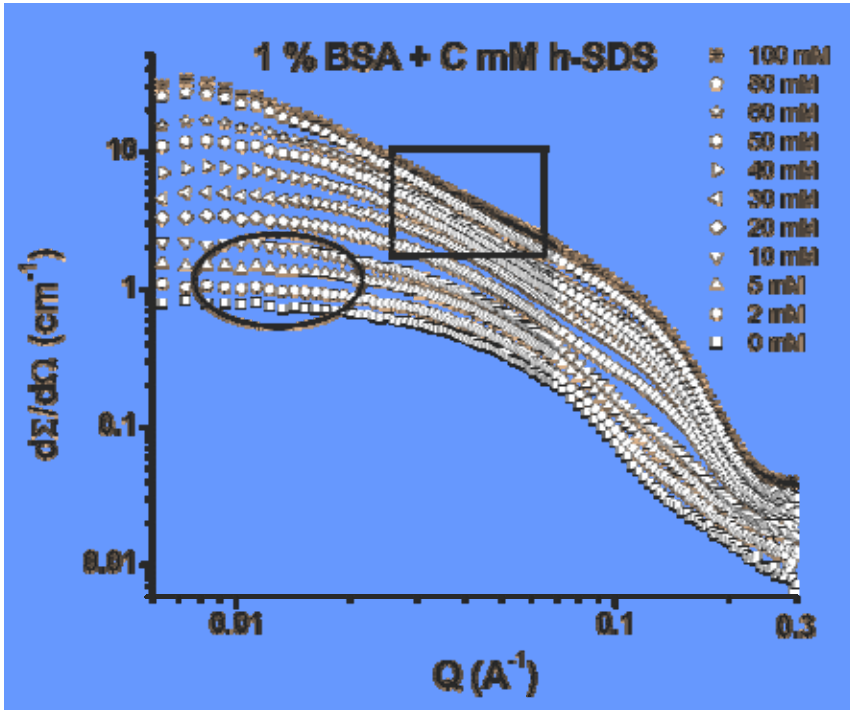
Protein Unfolding in Presence of Surfactant

PSI-BARC Collaboration

J. Kohlbrecher, R. Vavrin (LNS-PSI, Switzerland)

V.K. Aswal (BARC, Mumbai, India)

SANS data:

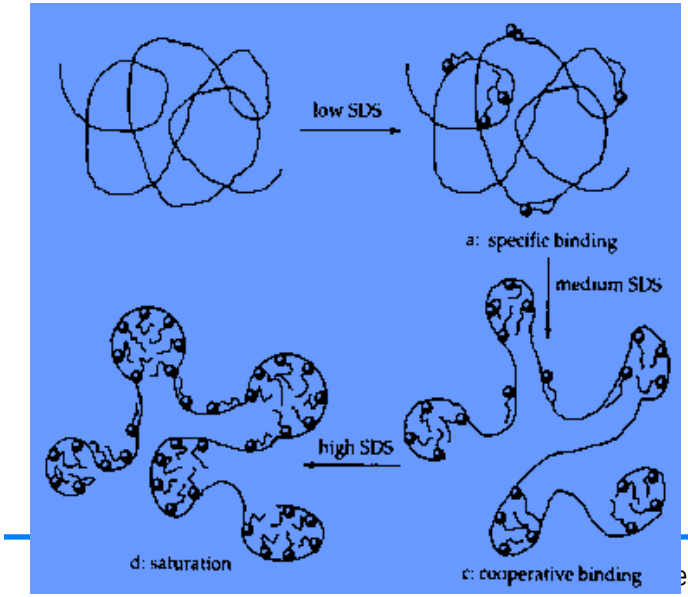


low surfactant concentration:

individual surfactant attach to deform the protein.
(deformation of protein)

high surfactant concentration:

micelle-like clusters of surfactants are formed along the unfolded polypeptide chain.
(fractal structure)

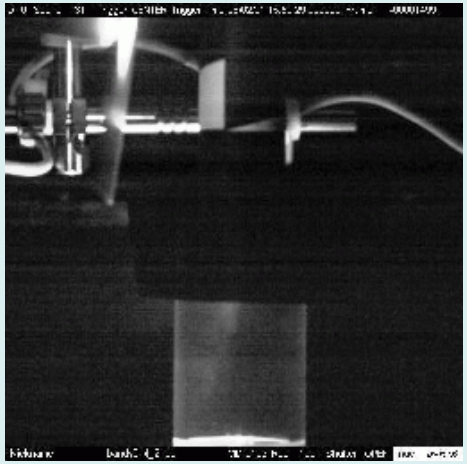


mechanism:

Alternating vorticity bands in a solution of wormlike micelles

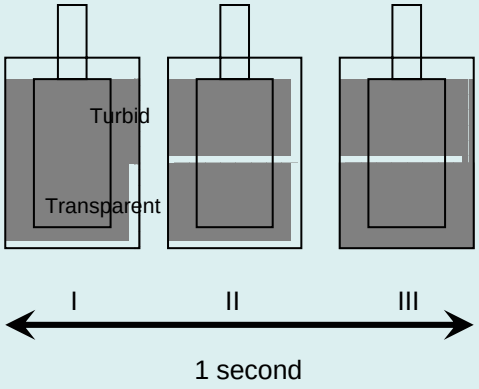
V. Herle[1], B. Pfister[1], P. Fischer[1], E.J. Windhab[1], and J. Kohlbrecher[2]

[1] Institute of Food Science, ETH Zurich
[2] Laboratory for Neutron Scattering, ETH Zurich & PSI



wormlike micelles are long, flexible, thread-like aggregates of surfactant molecules

- formation vorticity bands
- bands alternate in position
- shear rate and η show time dependent oscillations



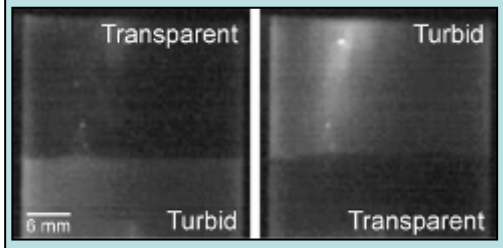
Problems and Questions

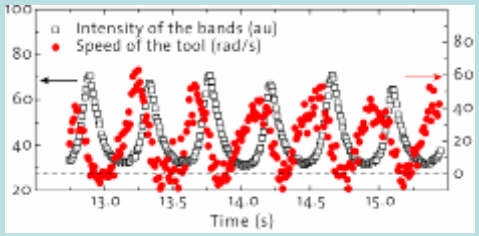
- How to capture the dynamics of the process
- Does the oscillation in the tool really corresponds to the bands?
- If yes, then, when does the tool slow down and when does it accelerate? (measuring the phase shift between structural change and shear rate oscillations)
- Which structures are formed in these bands?

Sept. '07, to be published in PRL

Rheology & Flow visualization

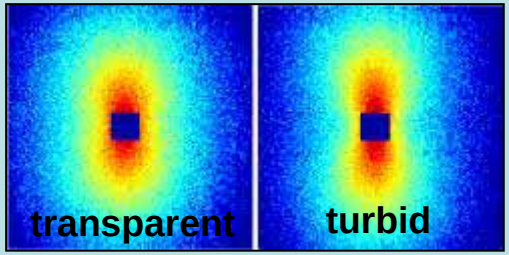
1. Stress controlled
2. Parallel plate or Couette
3. Steady and Transient

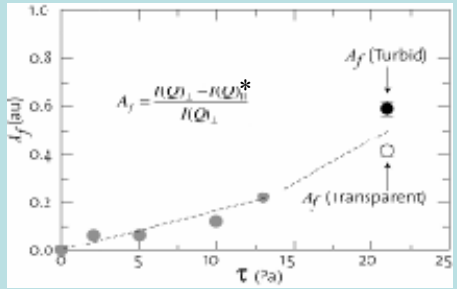




Rheo-Small Angle Neutron Scattering (Rheo-SANS)

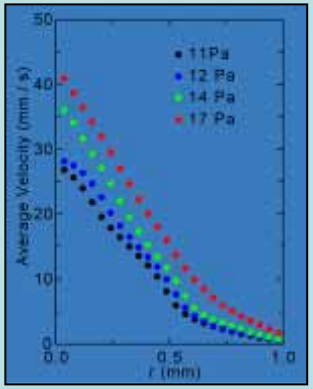
1. Stress controlled
2. Couette geometry
3. Triggered SANS





Ultrasound Velocity Profiling (UVP) and Rheo-NMR

1. Stress controlled
2. Couette geometry
3. Solution with tracer particles



Newtonian and shear thinning flow behavior with minor flow alignment of the micelles is observed. Above a critical stress of τ_c ~ 13 Pa shear thickening is observed with the formation of alternating transparent and turbid bands in the vorticity direction. Triggered SANS experiments show different anisotropic patterns in both bands indicating strongly aligned structures under flow. By video imaging experiments, we show that the pronounced shear-induced alignment of WMs in flow, does not correspond to a phase of lower viscosity.

J Kohlbrecher PSI

PAUL SCHERRER INSTITUT

Application of Avoided Level Crossing Muon Spin Resonance to Problems in Soft Matter Physics:

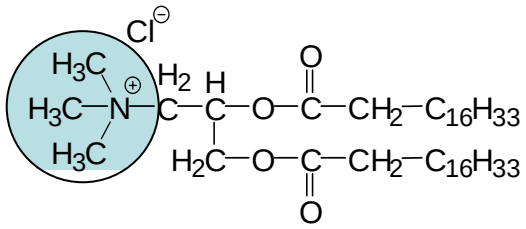
The Partitioning of Small Amphiphiles at the Bilayer/Water Interface in Lamellar Phase Dispersions

Collaboration PSI – Univ. Stuttgart – Unilever Research Port Sunlight

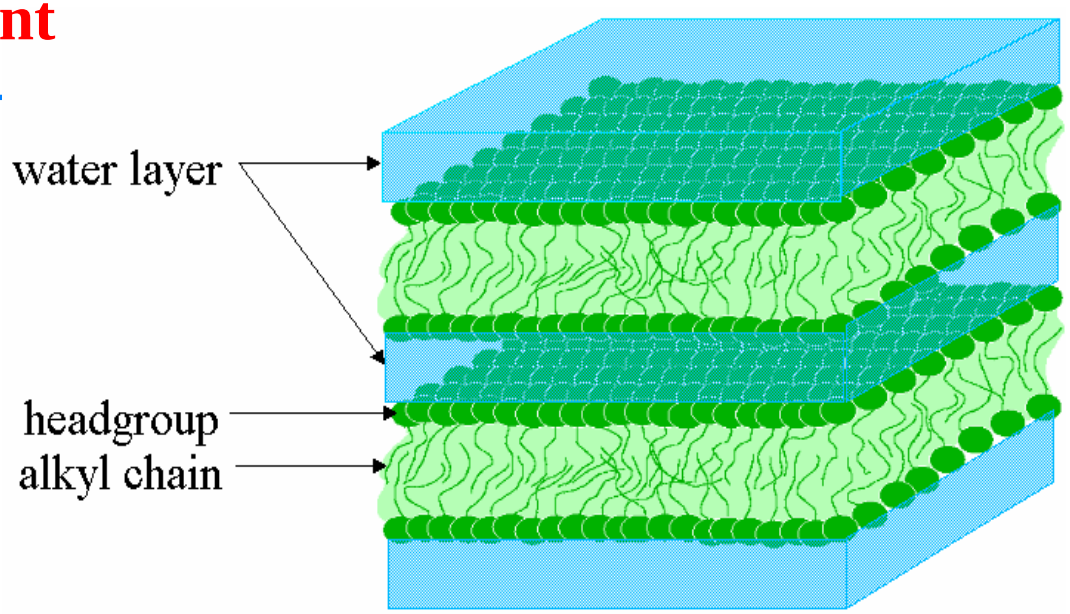
R. Scheuermann *et al.*, Phys. Chem. Chem. Phys. **4**, 1510 (2002)
R. Scheuermann *et al.*, accepted for publication in Langmuir (2004)

System: Detergent

lamellar phase:

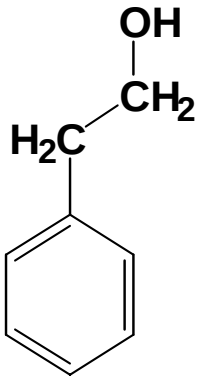


DHTAC: cationic dichain surfactant



surfactant bilayers separated by water

cosurfactant: 2-phenylethanol
('perfume': essence of roses)



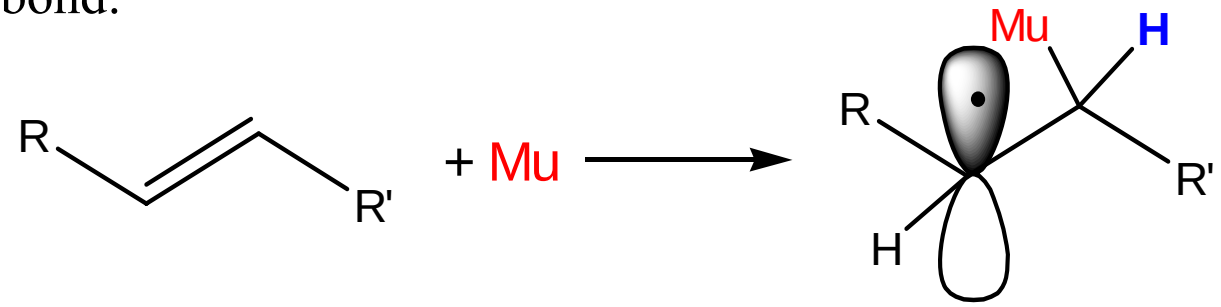
phase transition $T_{\alpha\beta} \approx 50$ °C (DSC)
$T > T_{\alpha\beta}$: L_α - alkyl chains ‚fluid'
$T < T_{\alpha\beta}$: L_β - more ordered packing of hydrocarbon chains

partitioning (local environment) of cosurfactants in lamellar phases

R. Scheuermann, PSI

Avoided Level Crossing μSR

formation of ≈100% polarised spin label by Mu addition to an unsaturated chemical bond:

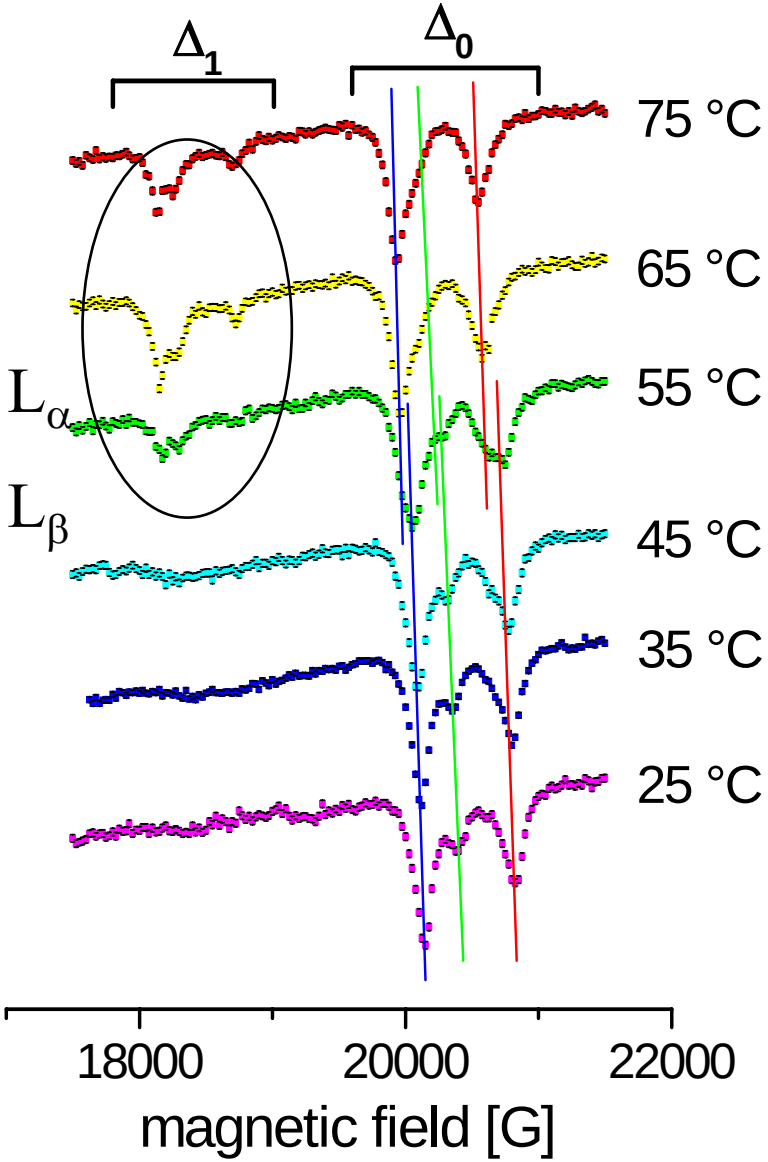


"Muon labeled Perfume"

3 spin-½ system: μ, p, e
Fermi contact interaction (electron spin density at muon/proton)
+ magnetic dipole interaction muon/proton – electron

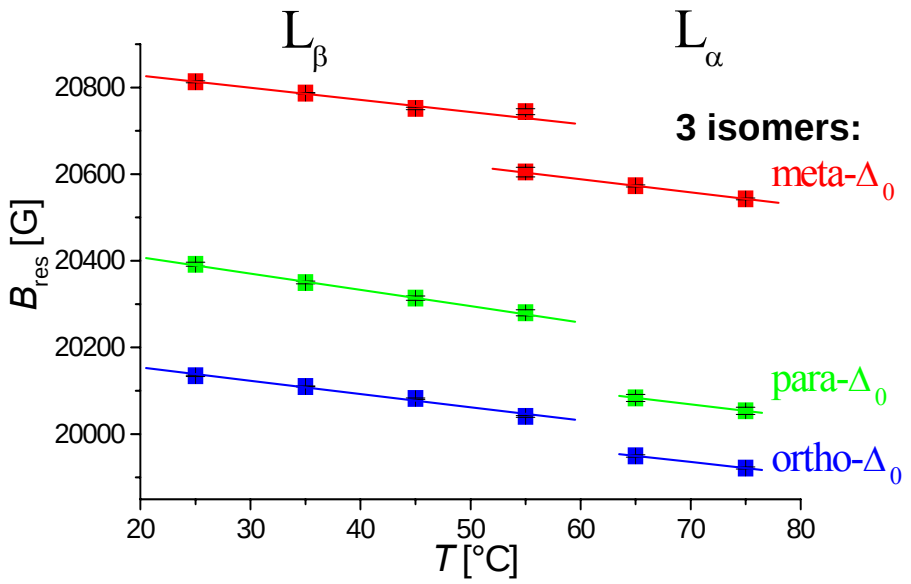
avoided crossings of magnetic energy levels at high magnetic fields (≈2 T)
⇒ dips in the field-dependence of the μ spin polarisation:
÷ longitudinal field relaxometry: spin-spin cross relaxation

40 mM 2-phenylethanol in 15% DHTAC dispersion



Δ_1 resonances only above $T_{\alpha\beta}$: residual anisotropy!
PEA-Mu axially aligned within bilayer
lineshape: dynamical averaging

Δ_0: discontinuity in $B_{res}(T)$ at $T_{\alpha\beta}$: **change of local environment!**



tracer **in water** **in bilayer**
(but not static!)

R. Scheuermann, PSI

Concentrated lamellar phase dispersion of surfactant (detergent)

Low concentration of cosurfactant (perfume), typ. 40 mM (100 µl/20 ml)

ALC-µSR:

spin-labelled perfume by Mu attachment

detection limit ≈1-10 µl/20 ml (10^{-4})

Lineshapes contains detailed information on dynamics …. But extraction of these details not straightforward.

Acknowledgements

NEUTRON SCATTERING & THE LIFE SCIENCES
Extracted from: "Neutron Scattering and the Life Sciences. A Strategy for the ILL" by P. A. Timmins

NEUTRONS IN BIOLOGY WORKSHOP

The Scientific and Technical Requirements for Biology at Australia's Replacement Research Reactor

The impact of neutrons on biological systems Olwyn Byron, University of Glasgow, Scotland, UK

Neutron diffraction studies of Escherichia coli dihydrofolate reductase complexed with methotrexate

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Enhanced visibility of hydrogen atoms by neutron crystallography on fully deuterated myoglobin

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Scientists from LNS – Diffraction, Reflectometry and SANS

Neutron and Muon portal – a key web-site

For information on and links to neutron and muon sources World-wide:

http://www.neutron-eu.net/

This site also contains information on how to get access to the European Facilities