

Small-angle scattering - the nuts and bolts

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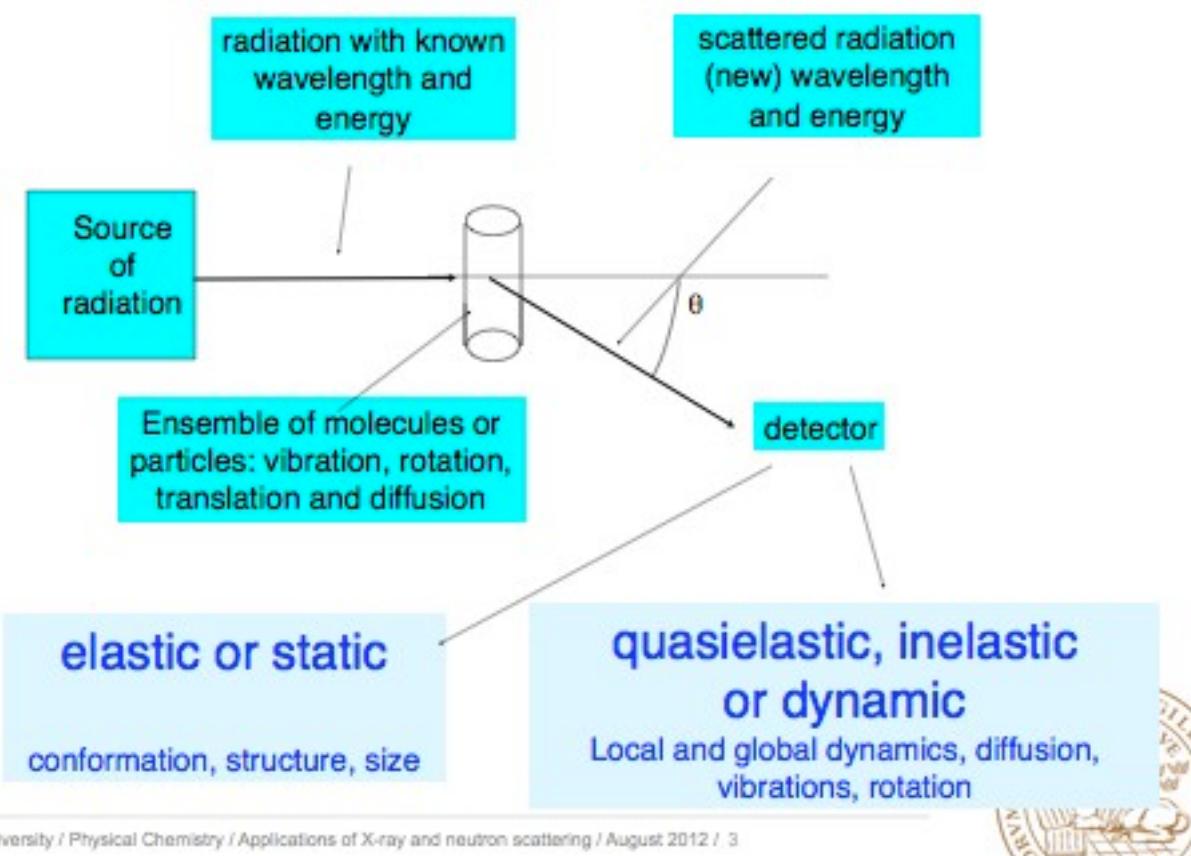
Contents

1. A short summary of scattering theory: Why SAS
2. Small-angle neutron scattering: Principles, instrumentation, resolution
3. Small-angle X-ray scattering: Principles and resolution
4. The concept of contrast and contrast variation
5. Selected soft matter examples



Recapitulation scattering methods

Probe choice: length and time scales, contrast



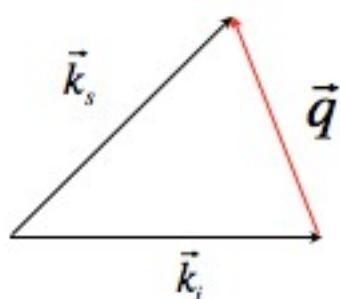
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Scattering methods - short repetition

Definition of the scattering vector \vec{q} :

$$\vec{q} = \vec{k}_s - \vec{k}_i$$

momentum transfer



Interference and scattering vector

scattering by N point scatterers at fixed positions

$$A_s(\vec{R}') = \sum_{j=1}^N A_j^s \cong \frac{A_0}{R'} e^{i\vec{k}_s \cdot \vec{R}'} \sum_{j=1}^N b_j e^{-i\vec{q} \cdot \vec{r}_j}$$

Fourier transform of $b(r)$

differential scattering cross section, identical particles:

$$\frac{d\sigma}{d\Omega}(\vec{q}) = \frac{\langle I_s(\vec{R}) \rangle}{I_0} R'^2 = b^2 \sum_{j,k=1}^N \langle e^{-i\vec{q} \cdot \vec{r}_{jk}} \rangle$$



Scattering cross section

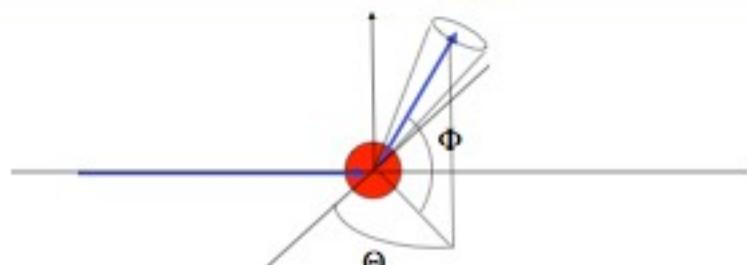
scattering cross section:

$$\text{scattering cross section } \sigma = \frac{\text{total scattered energy}}{\text{incident energy per area}}$$

Example billiard spheres: Cross section of sphere

differential scattering cross section:

$$\frac{d\sigma}{d\Omega} = \frac{\text{total scattered energy per solid angle } d\Omega \text{ (direction } \theta, \phi\text{)}}{\text{incident energy per area}}$$



The particle form factor

an „ideal gas“ of noninteracting particles:

$$I_s(q) = N \cdot I_p(q) = N \cdot I_p(0) \cdot P(q)$$

$I_p(0) = V^2 \Delta \rho^2$ intensity of single particle at $q = 0$

$P(q)$ particle form factor, where

$$P(q) = \frac{I_p(q)}{I_p(q \rightarrow 0)}$$

$P(q) \rightarrow$ contains information about size and structure of particle



Scattering from extended particle fixed in space II

resulting scattering amplitude of extended mobile particle in solvent:

particle in solvent:

excess scattering length density

$$\Delta \rho = \rho - \rho_{solv} = \frac{1}{V_1} \left(\sum_j b_j - \rho_{solv} V_1 \right)$$

average over all orientations:

$$\langle e^{i\vec{q} \cdot \vec{r}} \rangle = \frac{\sin qr}{qr}$$

$$I(q) = \langle A_s(\vec{q}) \cdot A_s^*(\vec{q}) \rangle = 4\pi \int_0^\infty \Delta \tilde{\rho}^2(r) r^2 \frac{\sin(qr)}{qr} dr$$

used spherical symmetry with $\Delta \rho(\vec{r}) = \Delta \rho(r)$

Loss of information \rightarrow 3-dim. structure of particle is represented by 1-dim.
function $I(q)$

$I(q)$ is function of magnitude of scattering vector $|\vec{q}|$



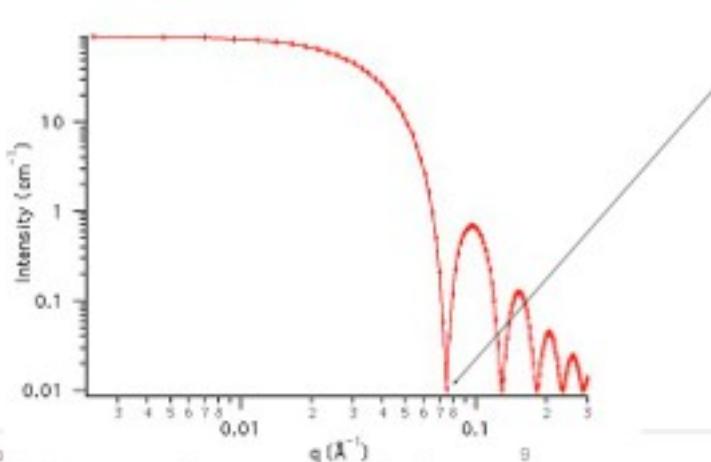
The particle form factor II

Example: homogeneous sphere

$$P(q) = \left[3 \left(\frac{\sin(qR) - (qR)\cos(qR)}{(qR)^3} \right) \right]^2$$

function has minima for $\tan(qR) = qR$, or $qR = 4.49, 7.73, \dots$

calculation for sphere with radius $R = 60 \text{ \AA}$ \rightarrow minima at $q = 4.49/60 = 0.075$



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The structure factor S(q)

Scattering intensity from an ensemble of identical particles with scattering amplitude $A_i(q)$ and position r_i :

$$\frac{d\sigma}{d\Omega}(q) = \sum_{j,k=1}^N \left\langle A_j(q) A_k(q) e^{-i\vec{q} \cdot (\vec{r}_j - \vec{r}_k)} \right\rangle = N I_p(0) P(q) S(q)$$

Static structure factor $S(q)$:

$$S(q) = \frac{1}{N} \sum_{j,k=1}^N \left\langle e^{-i\vec{q} \cdot (\vec{r}_j - \vec{r}_k)} \right\rangle$$

Scattering intensity from an "ideal gas" of noninteracting particles:

$$\left[\frac{d\sigma}{d\Omega}(q) \right]_{i.g.} = N A(0)^2 P(q)$$

-> $S(q)$ contains information about particle correlations due to interactions:

$$S(q) = \frac{\left[\frac{d\sigma}{d\Omega}(q) \right]}{\left[\frac{d\sigma}{d\Omega}(q) \right]_{i.g.}}$$



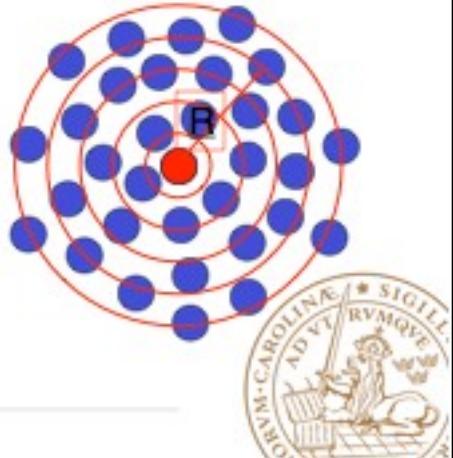
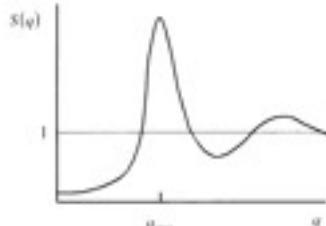
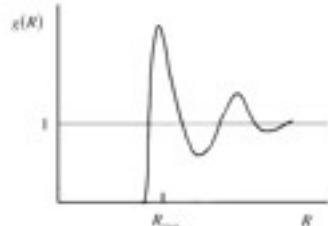
Interacting particles: the structure factor $S(q)$

radial distribution function $g(r)$ as a measure of spatial correlation:

$$\rho g(\vec{r}) = \frac{1}{N} \left\langle \sum_{j=1}^N \sum_{k=1}^N \delta(\vec{r} - \vec{r}_{jk}) \right\rangle$$

number of particles in volume element dV at a distance r from given particle: $\rho g(r) dV$

$$S(q) = 1 + 4\pi\rho \int_0^\infty [g(r) - 1] r^2 \frac{\sin qr}{qr} dr$$

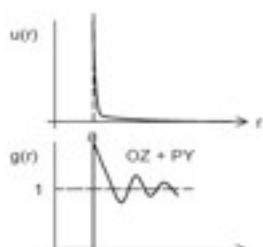


$$q_{\max} R_{\max} \approx 2\pi$$

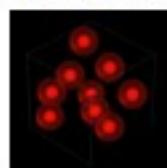
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Interacting particles: the structure factor $S(q)$ II

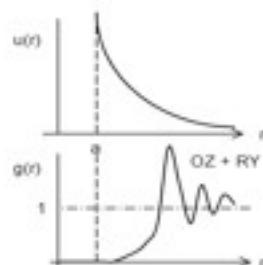
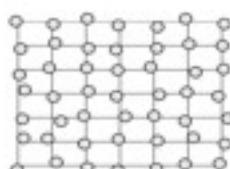
Hard Spheres



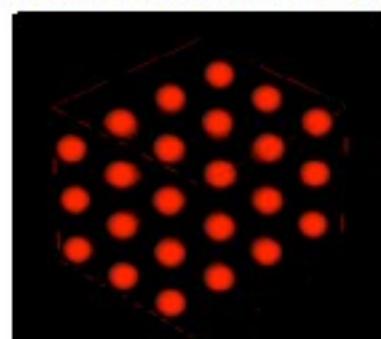
* Correlated liquids
short-range correlations



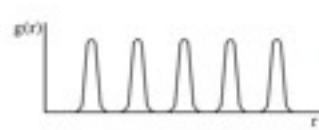
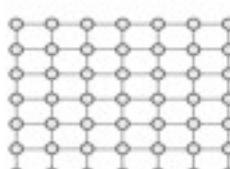
Charged Spheres



* Strongly correlated liquids
intermediate correlation range



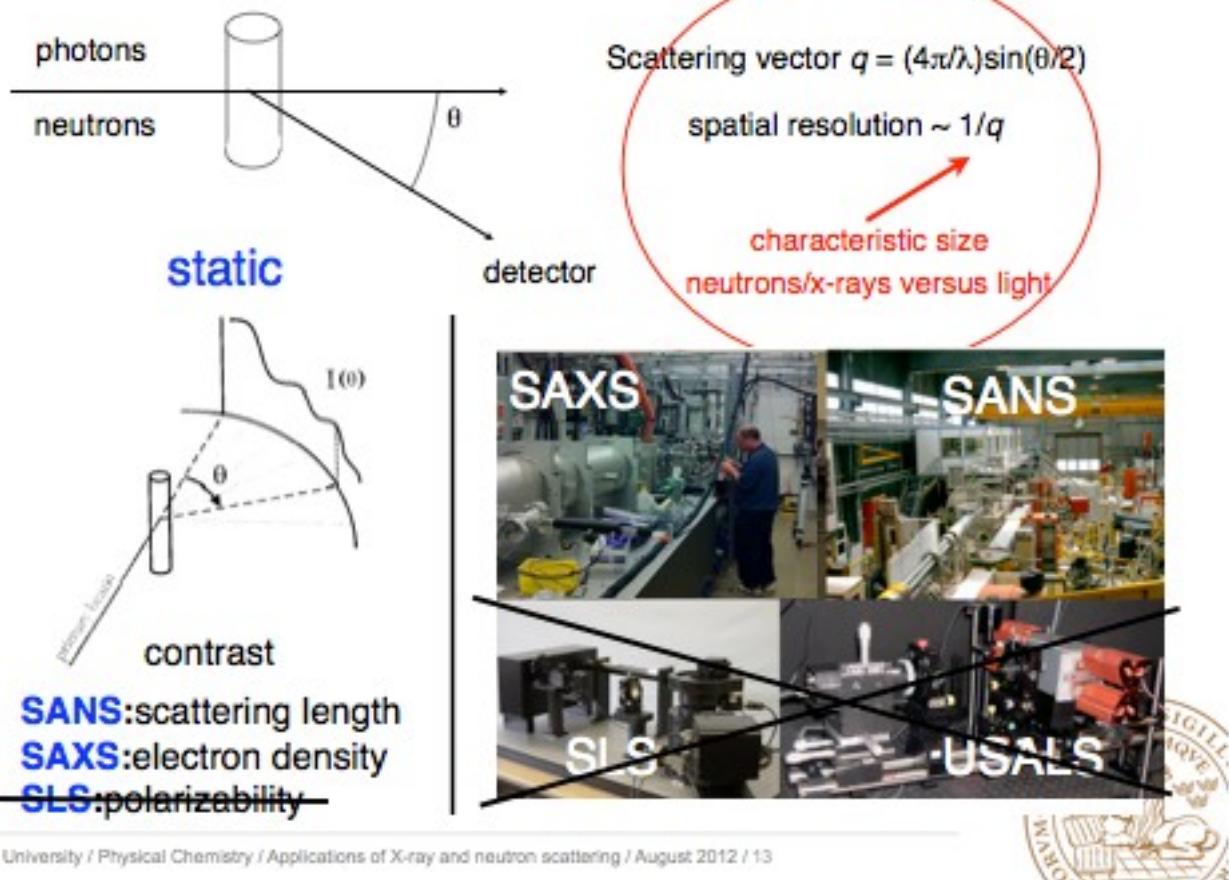
Crystal



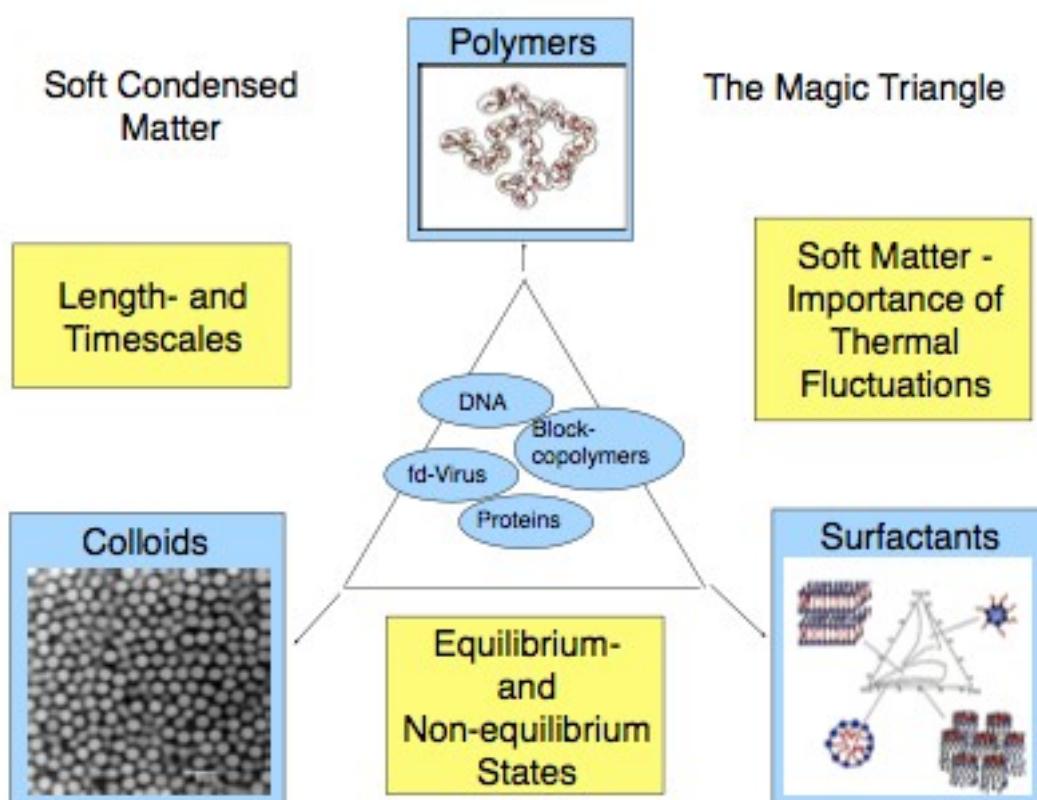
* Crystal
long-range correlations

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Scattering methods - short repetition



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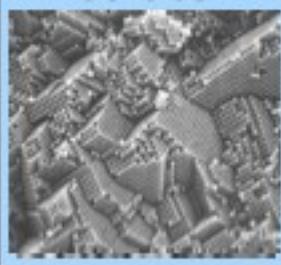


Soft Condensed Matter

Quantum dots for diagnostics and therapy



Colloids

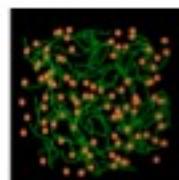


Polymers

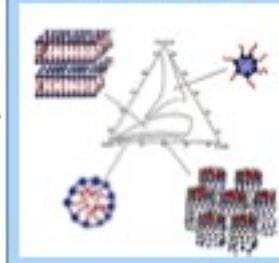


The Magic Triangle in Soft Nanotechnology

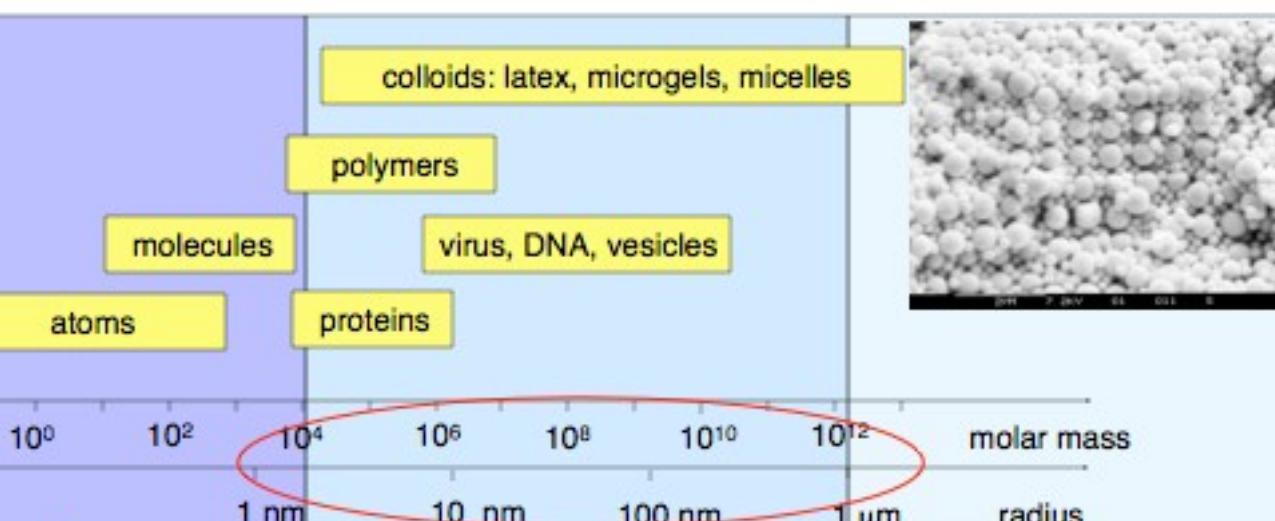
Nanocomposites with improved properties



Surfactants



Example Soft Matter: Characteristic length scales

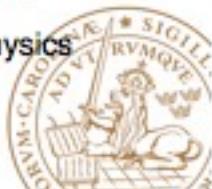


How do we investigate these structural details?

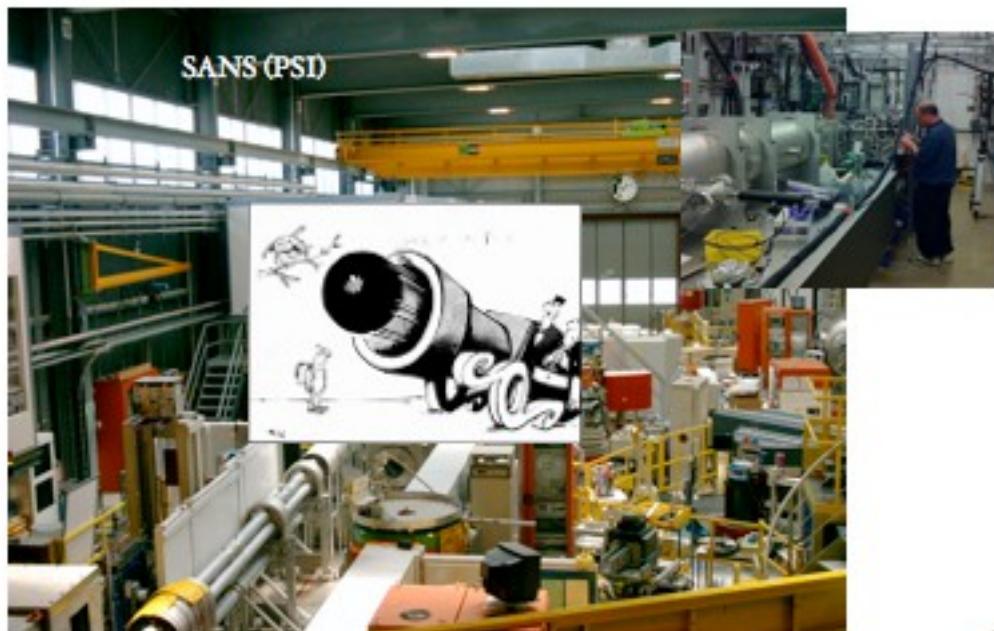
microscopic
atomic/molecular
physics and chemistry

mesoscopic
colloid physics and chemistry,
biology

macroscopic systems
solid state physics



Why SANS/SAXS when working with Softs Matter?



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Magnetic nanoparticles - a fascinating playground



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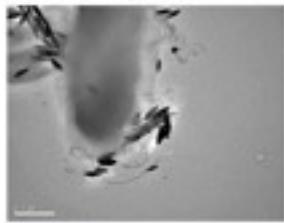
Magnetic nanoparticles

Fascinating materials

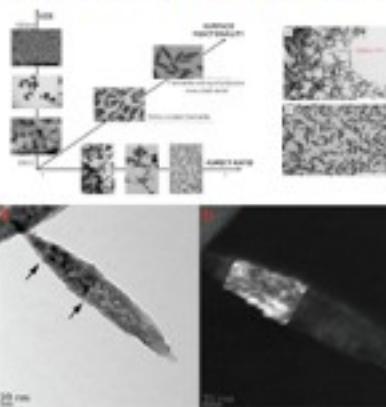
magnetorheological fluids



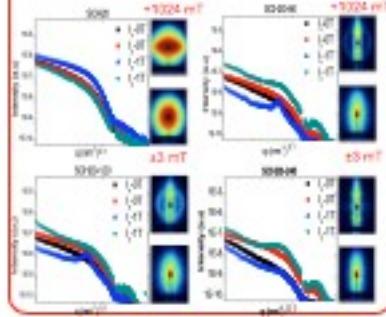
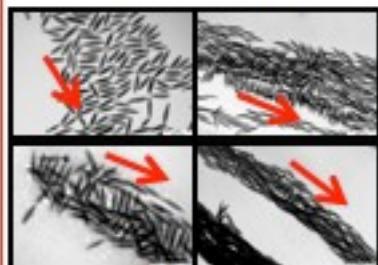
Fishing bacteria



Controlled synthesis of iron oxide magnetic particles



Magnetic field driven self-assembly



HOW DO WE STUDY THEM



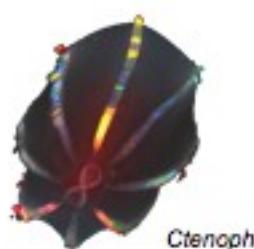
M. Reufer et al, J. Phys. Cond. Mat. (2011)

I. Martchenko et al, J. Phys. Chem. B (2011)

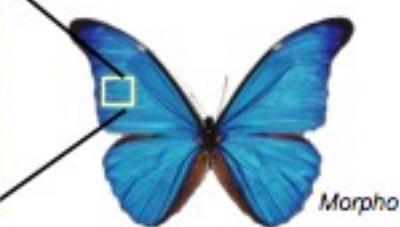
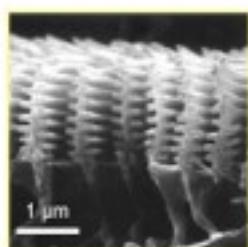
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Photonic materials through colloidal self assembly



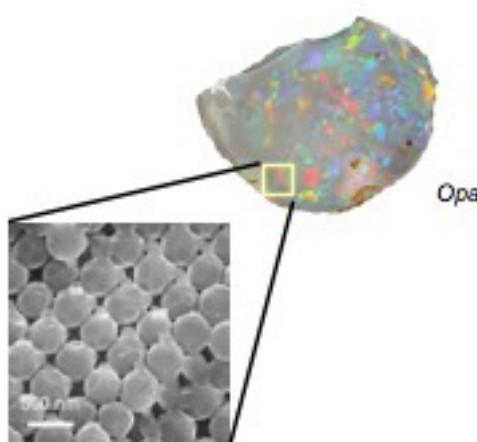
Ctenophora



Morpho



Peacock

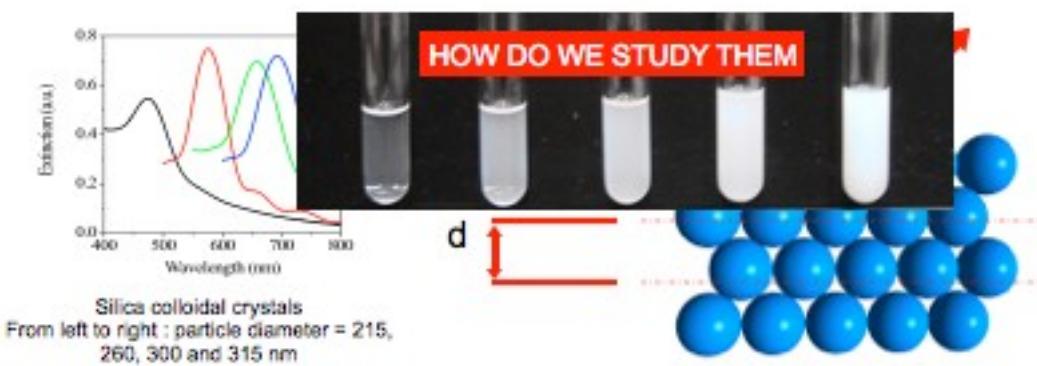
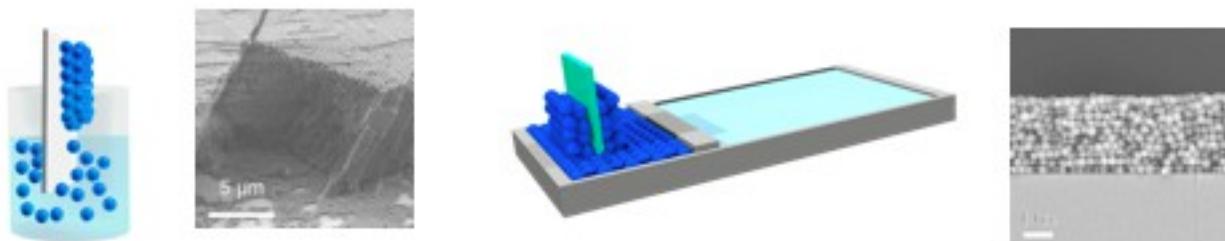


Opal



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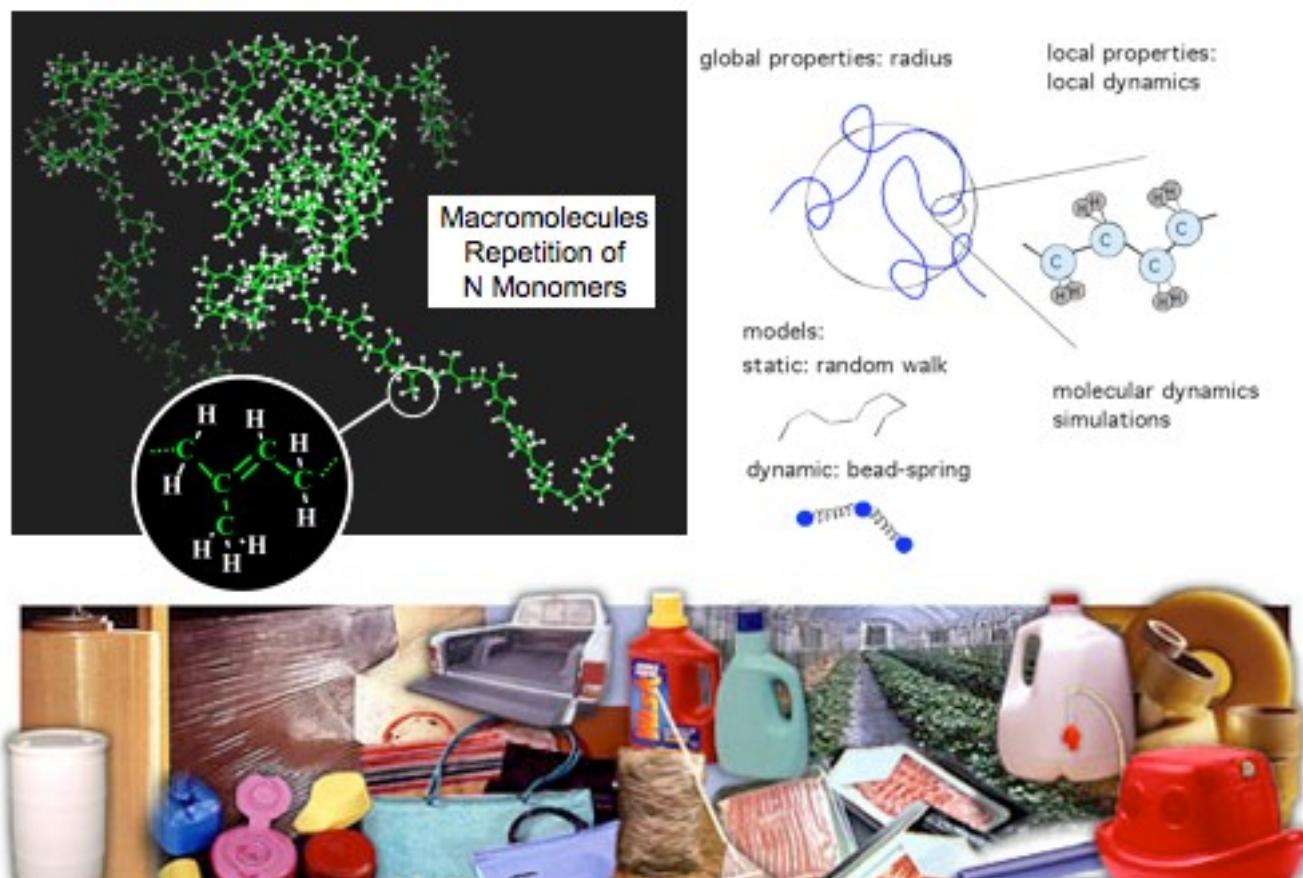
Photonic materials through colloidal self assembly



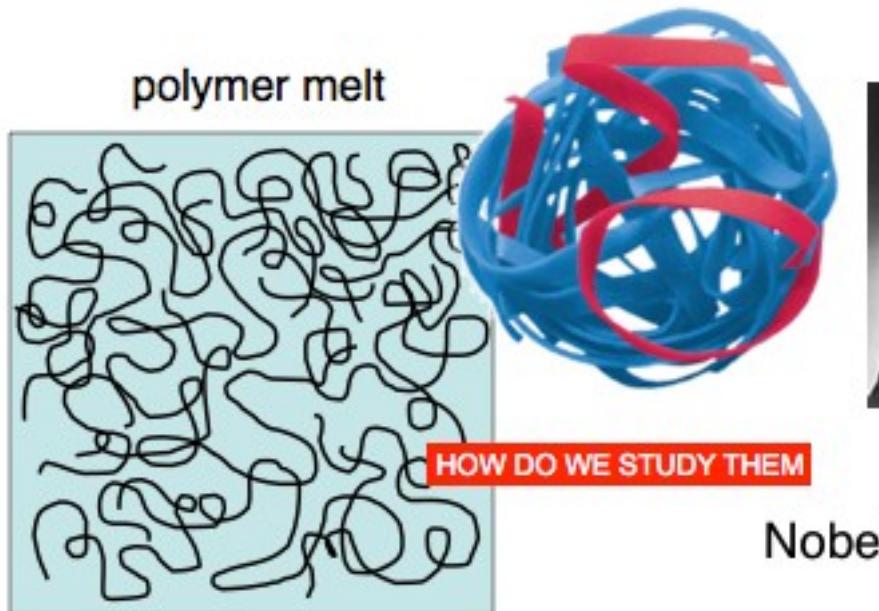
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Polymers - From the physicists dream objects to household utensils



How does a polymer look in the melt



P.J. Flory
Stanford
USA

Nobel prize 1974



Why SANS/SAXS

SANS/SAXS:

- appropriate length scales
- no multiple scattering (SAXS)
- avoid multiple scattering through contrast adjustment (SANS)
- create/vary contrast (mainly SANS)
- large penetration depth (SANS)
- weak interaction (SANS)

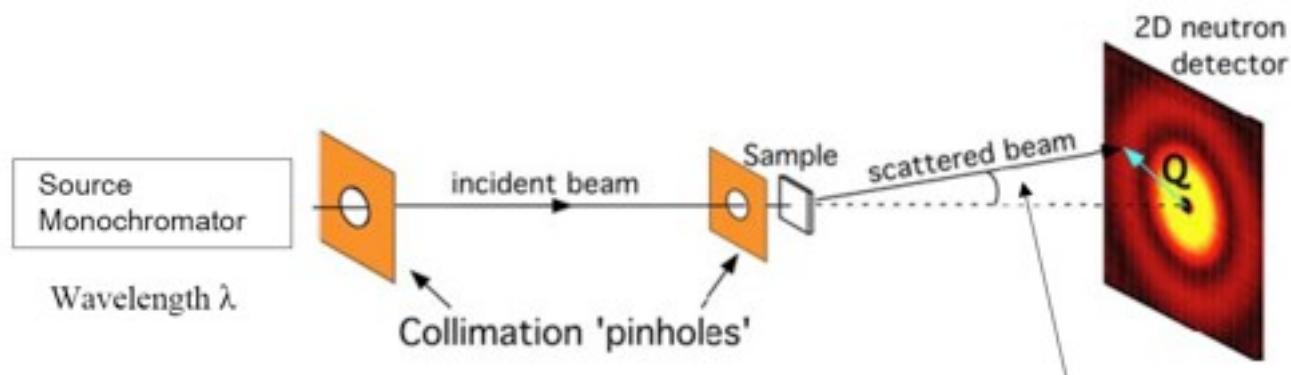


Contents

1. A short summary of scattering theory: Why SAS
2. Small-angle neutron scattering: Principles, instrumentation, resolution
3. Small-angle X-ray scattering: Principles and resolution
4. The concept of contrast and contrast variation
5. Selected soft matter examples



Small-angle scattering: The nuts and bolts



$$q \equiv 4\pi \sin\theta / \lambda$$

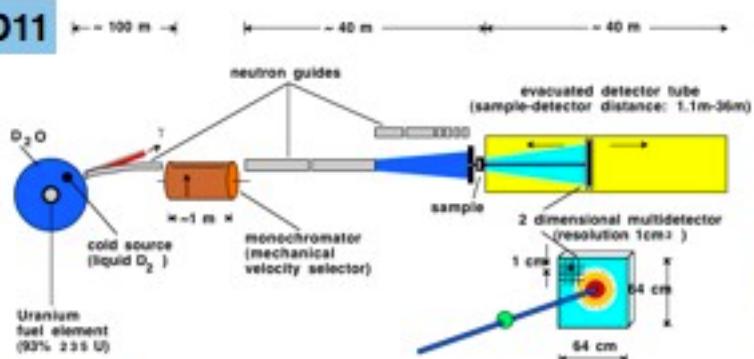
- Instrumental smearing
- SANS instrumentation
- SAXS instrumentation

Keywords:
Long-slit
Pin-hole
Focussing



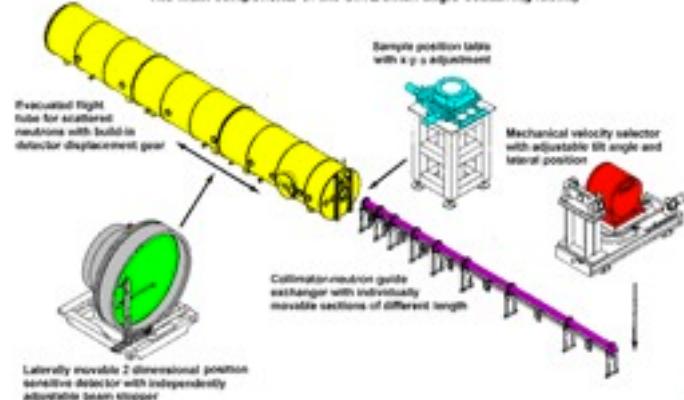
SANS instrumentation

ILL: D11



PSI: SANS1

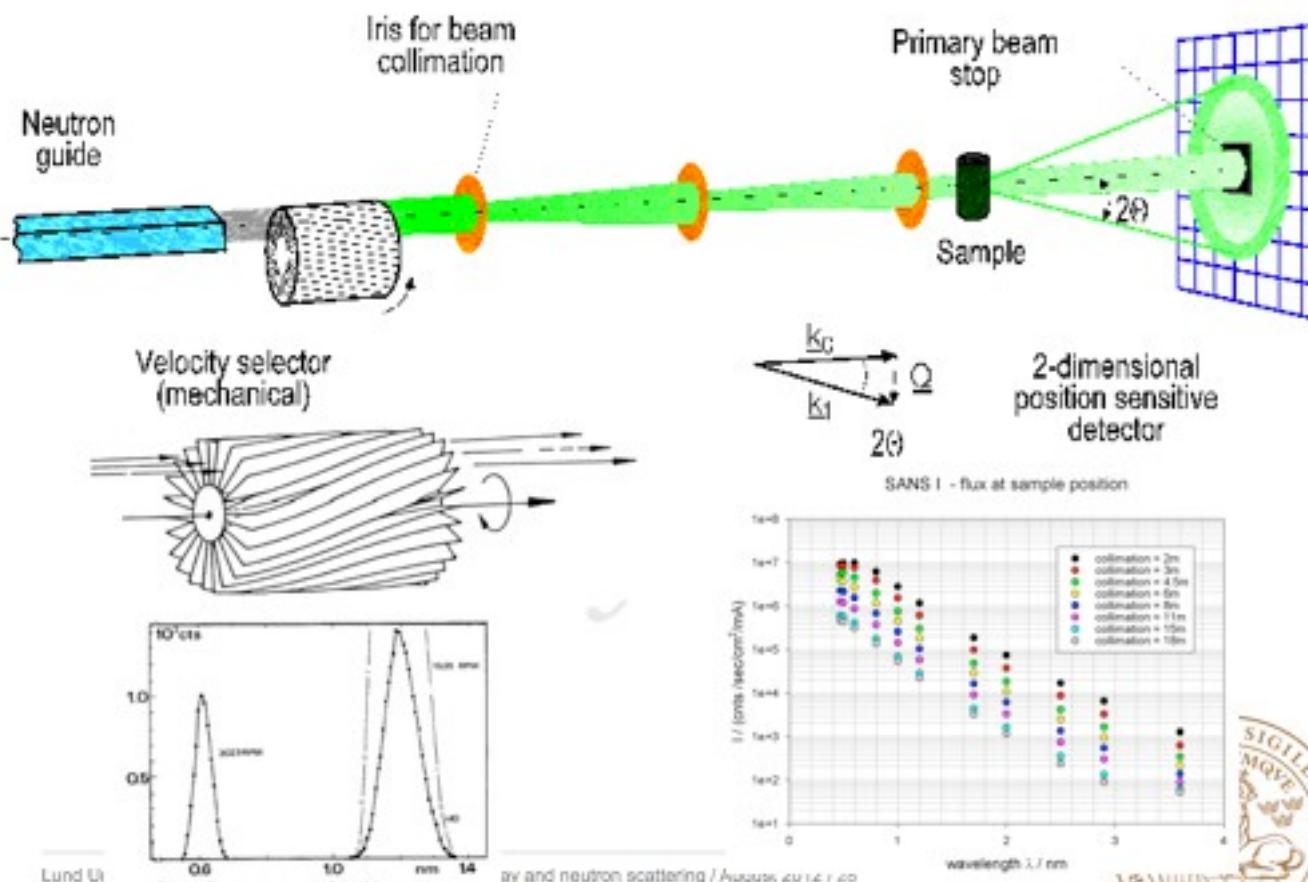
The main components of the SINQ small angle scattering facility



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SANS instrumentation

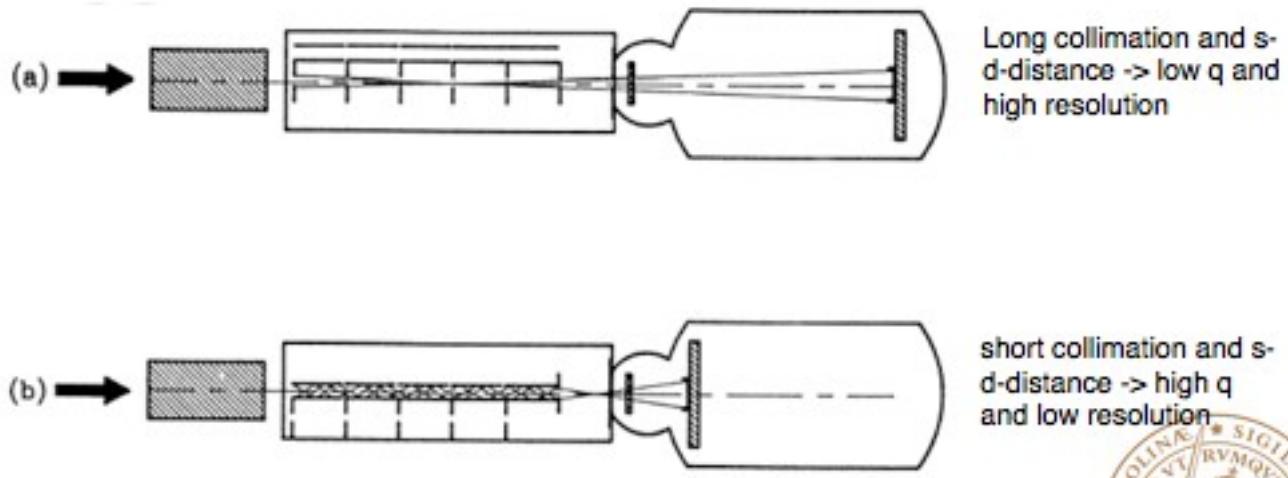


SANS: q-range and resolution

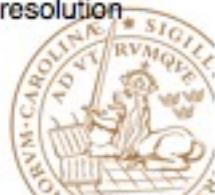
Low q – high q

0.001 – 0.5 1/Å

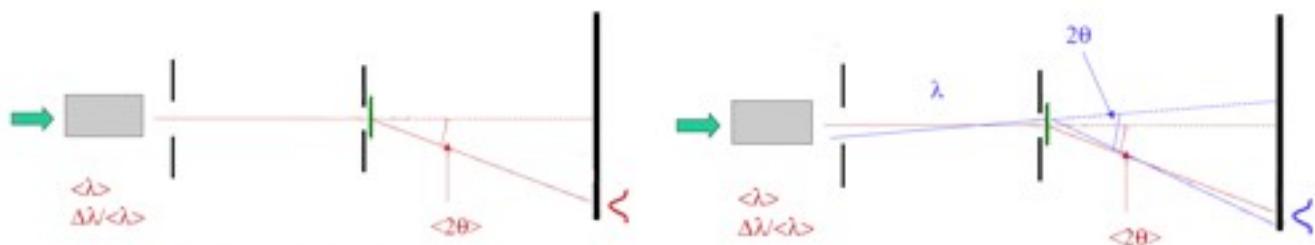
$\lambda = 3 - 30 \text{ \AA}$



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SANS: Resolution function and instrumental smearing



$$q = 4\pi \sin \theta / \lambda$$

Derivative with respect to λ :

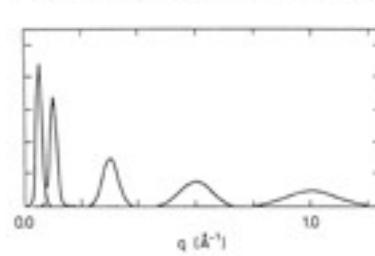
$$\Delta q = -q \Delta \lambda / \lambda$$

Derivative with respect to θ :

$$\Delta q = \frac{4\pi}{\lambda} \cos \theta \Delta \theta \approx \frac{4\pi}{\lambda} \Delta \theta$$

Assume independent distributions described by Gaussians:

$$\sigma(\langle q \rangle)^2 = \langle q \rangle^2 \sigma(\Delta \lambda / \lambda)^2 + (4\pi / \lambda)^2 \sigma(\Delta \theta)^2$$



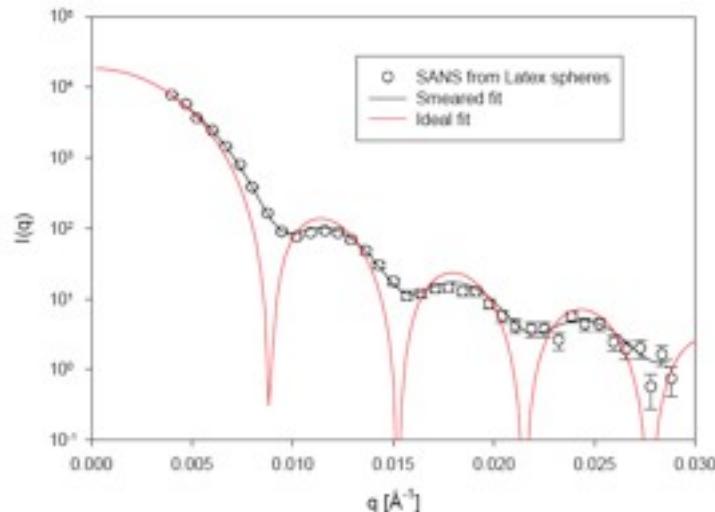
$$I(\langle q \rangle) = \int R(\langle q \rangle, q) \frac{d\sigma(q)}{dq} dq$$



SANS: Resolution function and instrumental smearing

Analysis with smearing

$$I(\langle q \rangle) = \int R(\langle q \rangle, q) \frac{d\sigma(q)}{d\Omega} dq \quad \frac{d\sigma}{d\Omega}(q) = \Delta\rho^2 V^2 \left[\frac{3[\sin(qR) - qR \cos(qR)]}{(qR)^3} \right]^2$$



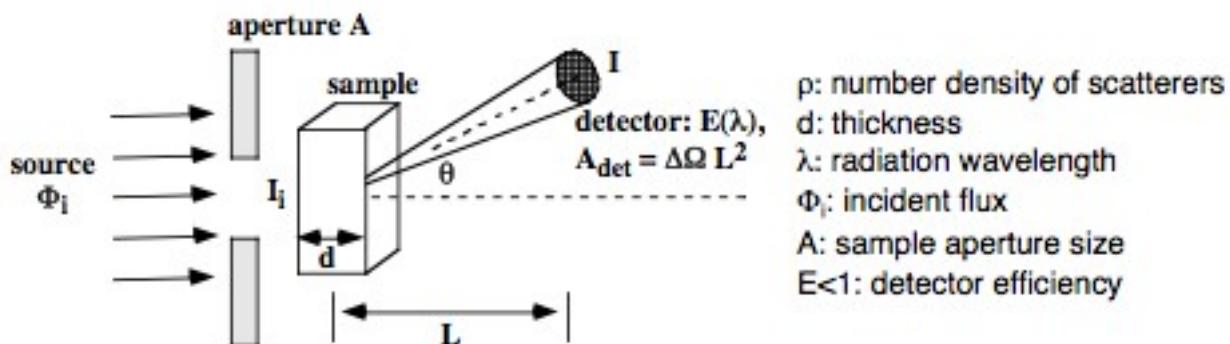
Lund

Data from Wiggnal et al.



SANS: Initial data treatment

Experimental intensity <-> scattering cross section



$$\text{incident intensity: } I_i [\text{s}^{-1}] : \Phi_i \cdot A \cdot E$$

attenuation before collision at $0 \leq x \leq d$: $\exp(-\mu x)$
collision (scattering) at x with probability $d\sigma/d\Omega$
attenuation after collision at $0 \leq x \leq d$: $\exp(-\mu(d-x))/\cos\theta$

Integration along x , through the sample, with $\cos\theta \approx 1$ (SAS)

$$\Rightarrow I(\theta) = \underbrace{\Phi_i E \Delta\Omega A d}_{C(\lambda)} \exp(-\mu d) \rho \frac{d\sigma}{d\Omega}$$

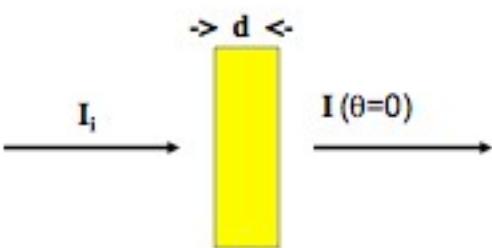


SANS: Initial data treatment - Transmission

attenuation of incident intensity due to scattering, absorption:

$$T_s = I(\theta=0) / I_i = \exp(-\mu d) = \exp(-d/\Lambda)$$

(I_i, I measured under identical conditions !)



μ [cm⁻¹]: linear attenuation coefficient

Λ [cm] = $1/\mu$ = mean free path of radiation before collision

from $I(\theta) = C(\lambda) d T d\Sigma/d\Omega$

=> $I \sim d T$ is maximum for $d = 1/\mu = \Lambda$

but multiple scattering is minimum for $d \ll \Lambda$

=> look for a compromise (small d preferred)

X-rays: μ = absorption coefficient

μ_{abs} , absorption is essential part of attenuation

Δ_λ : 0.01 mm - 1 mm

Neutrons: $\mu = \mu_{coh} + \mu_{abs} + \mu_{inc}$

$\mu = \Sigma$ "total scattering cross section"

Δ_n : 0.5 mm - 10 mm

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SANS: Initial data treatment - Background

Background correction

measured I^m_{S+SB} (e.g. polymer solution) : background !

=> need I_s : corrected for external background

- A. scale to incident beam monitor,
correct relative efficiencies of detector "cells"
- B. 1. Sample in container I^m_{S+SB}
2. Empty container scattering I^m_{SB}
3. Room background, electronic noise I^m_{Cd}

$$\Rightarrow I_s = [(I^m_{S+SB} - I^m_{Cd}) / T_{S+SB} - (I^m_{SB} - I^m_{Cd}) / T_{SB}]$$

same treatment to be applied for reference (solvent sct.)



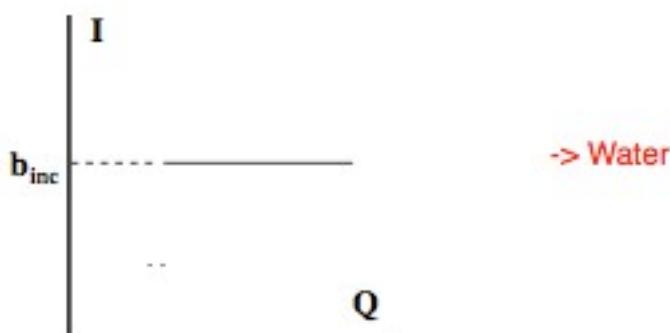
SANS: Absolute calibration

use of standard samples with well known $(d\Sigma/d\Omega)_{St}$

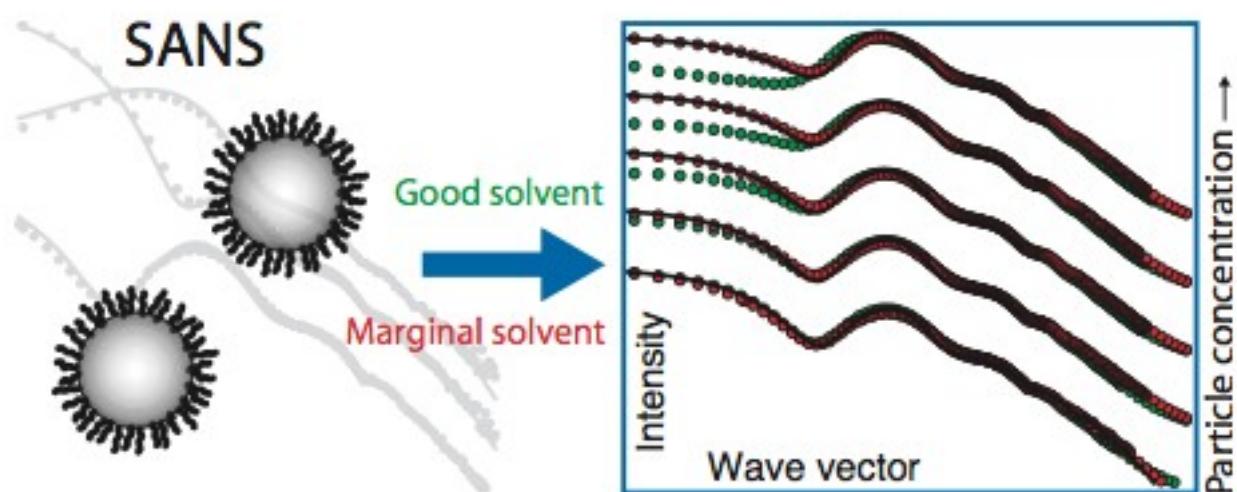
$$d\Sigma/d\Omega = [I_{St} \cdot T_{St}/(I_{St} \cdot dT)] \cdot (d\Sigma/d\Omega)_{St}$$

Incoherent scattering

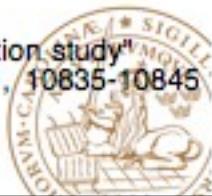
$$(d\Sigma/d\Omega)_{St} = \rho \cdot (b_{inc})^2 = \text{constant}$$



Data treatment example: Sterically stabilized colloidal particles



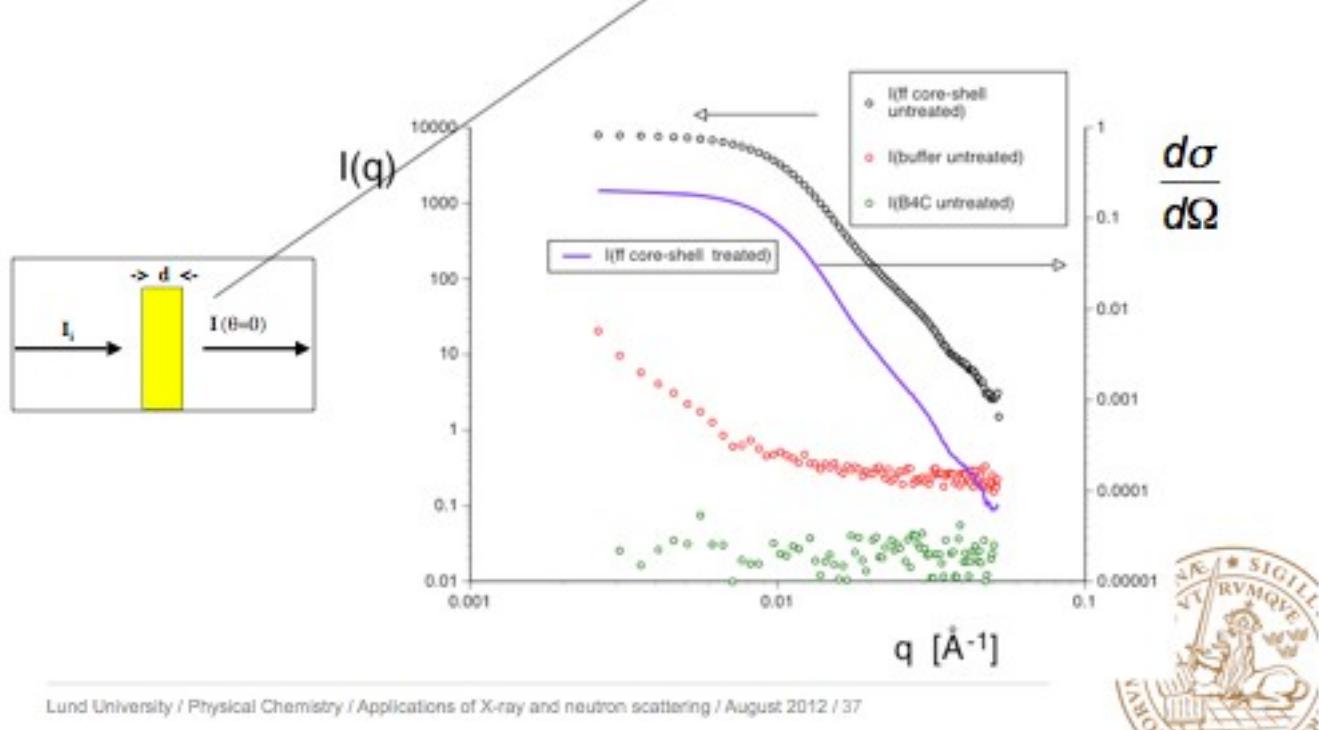
"Small-angle neutron scattering on a core-shell colloidal system: a contrast-variation study"
M. Zackrisson, A. Stradner, P. Schurtenberger, and J. Bergenholz, Langmuir 21, 10835-10845
(2005)



Initial data treatment low-q

Example form factor measurement on D22: det 17.6 m, coll 17.6 m, $\lambda = 7\text{\AA}$

$$\Rightarrow I_s = [(I^m_{S+SB} - I^m_{Cd})/T_{S+SB} - (I^m_{SB} - I^m_{Cd})/T_{SB}]$$



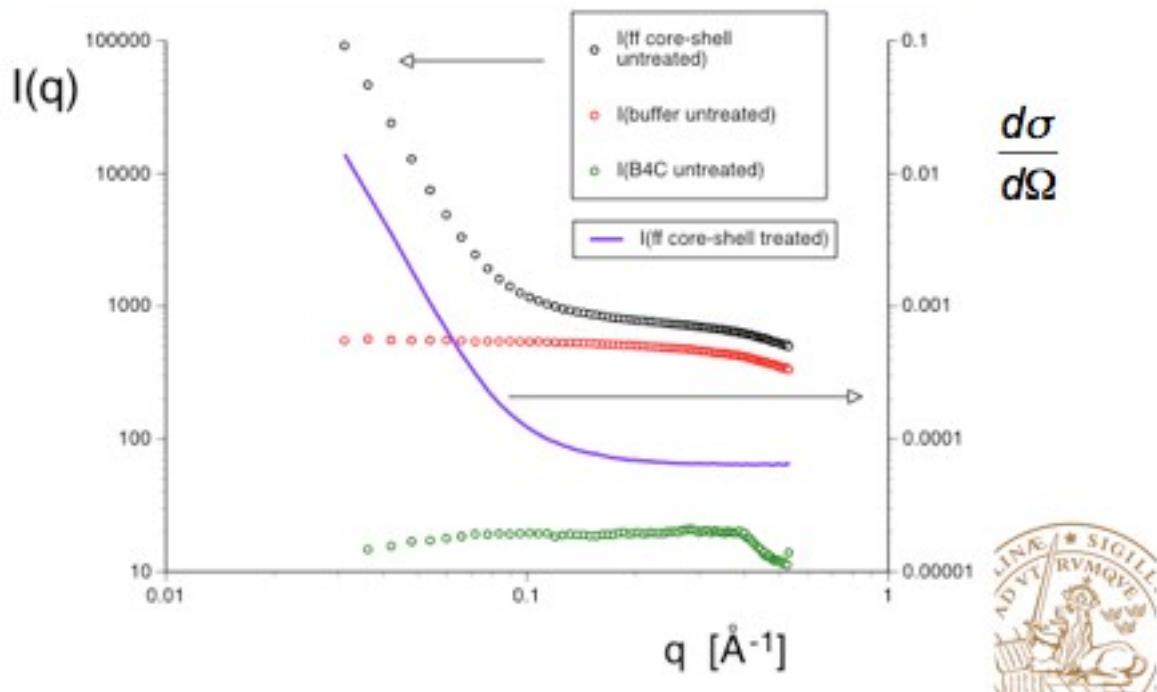
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Initial data treatment high-q

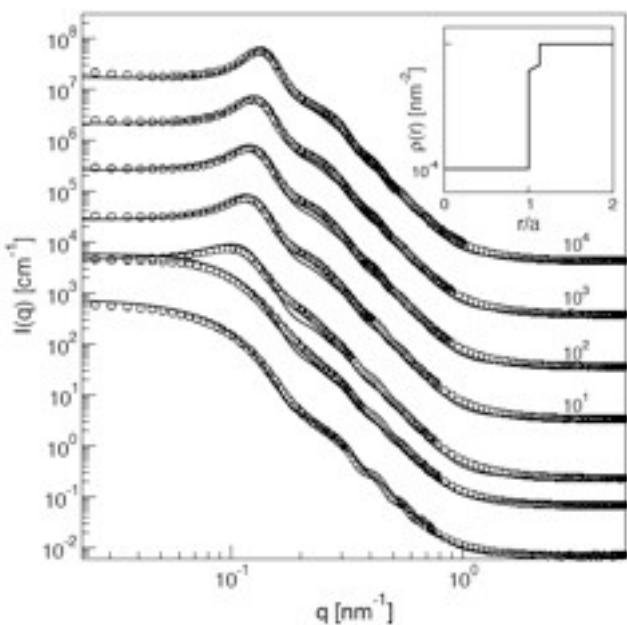
Example form factor measurement on D22: det 1.5 m, coll 4 m, $\lambda = 7\text{\AA}$

$$\Rightarrow I_s = [(I^m_{S+SB} - I^m_{Cd})/T_{S+SB} - (I^m_{SB} - I^m_{Cd})/T_{SB}]$$



SANS: final treated data

Example colloid concentration series on D22:



"Small-angle neutron scattering on a core-shell colloidal system: a contrast-variation study"
M. Zackrisson, A. Stradner, P. Schurtenberger, and J. Bergenholtz, Langmuir 21, 10835-10845
(2005)

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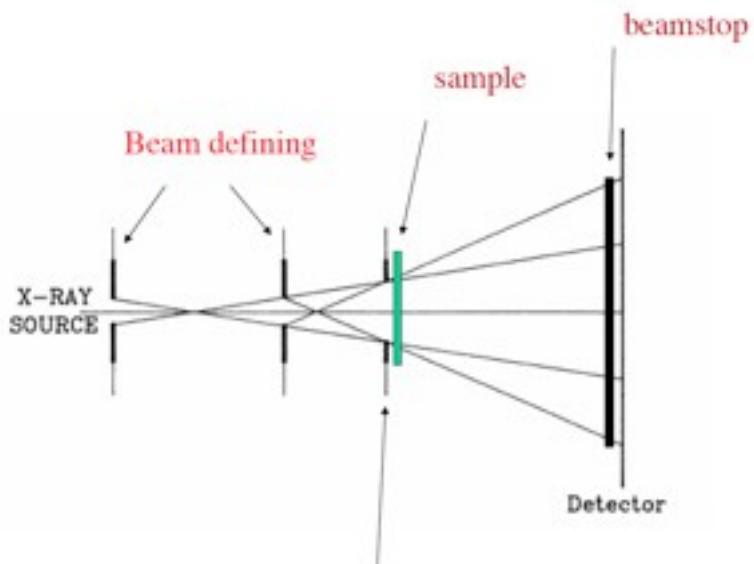


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1. A short summary of scattering theory: Why SAS
2. Small-angle neutron scattering: Principles, instrumentation, resolution
- 3. Small-angle X-ray scattering: Principles and resolution**
4. The concept of contrast and contrast variation
5. Selected soft matter examples



SAXS instrumentation



simplest system: pair of 2 parallel slits

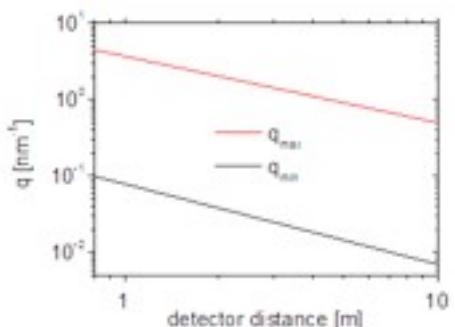
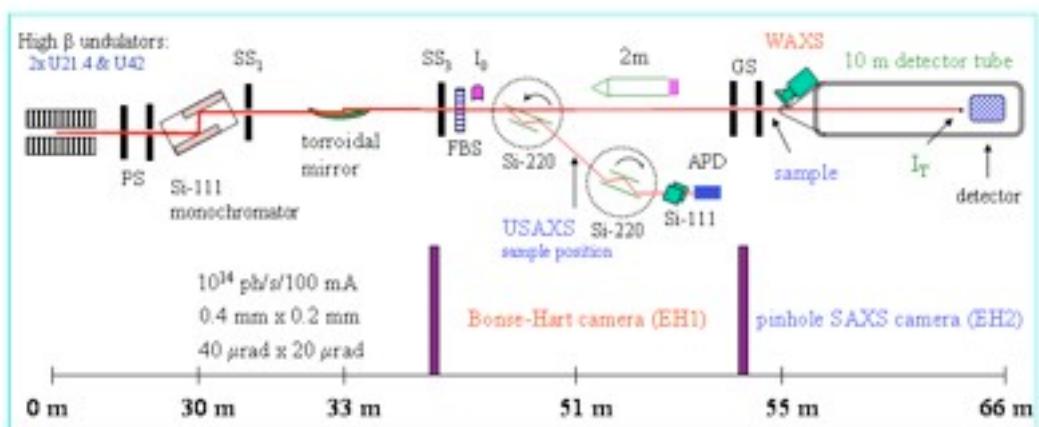
* problem: each edge → gives rise to secondary radiation (= parasitic scattering)

* third slit → removes parasitic scattering of the 2nd slit (must not touch the intensive, direct primary beam!)

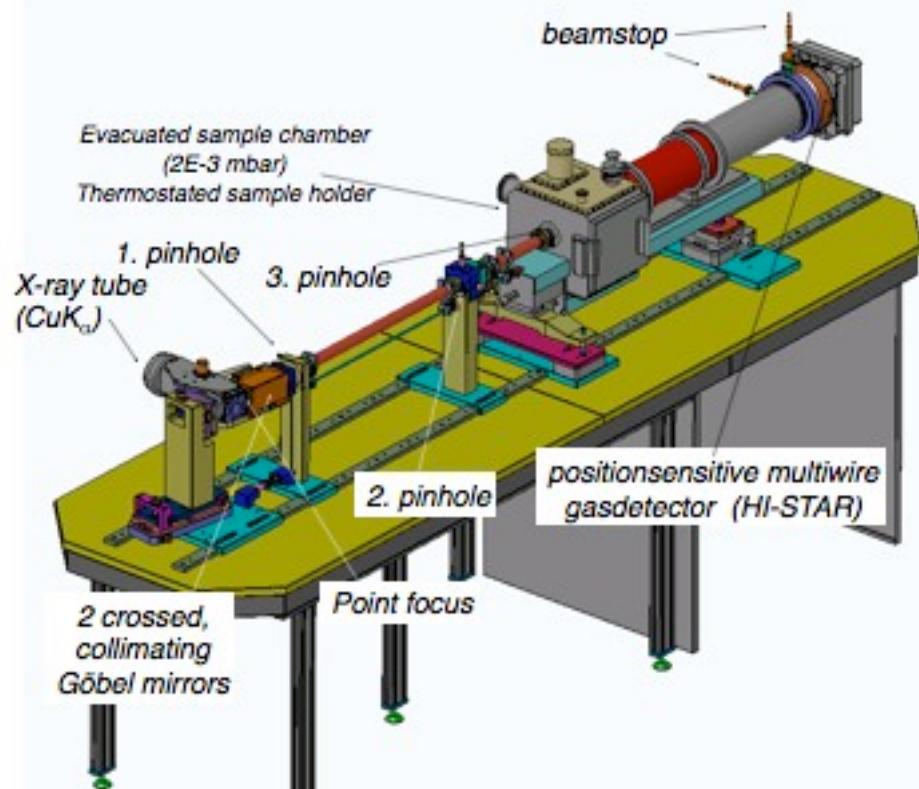
Guard pinhole/slit or anti-scatter pinhole/slit



SAXS at ESRF: ID2



SAXS: Laboratory pinhole camera



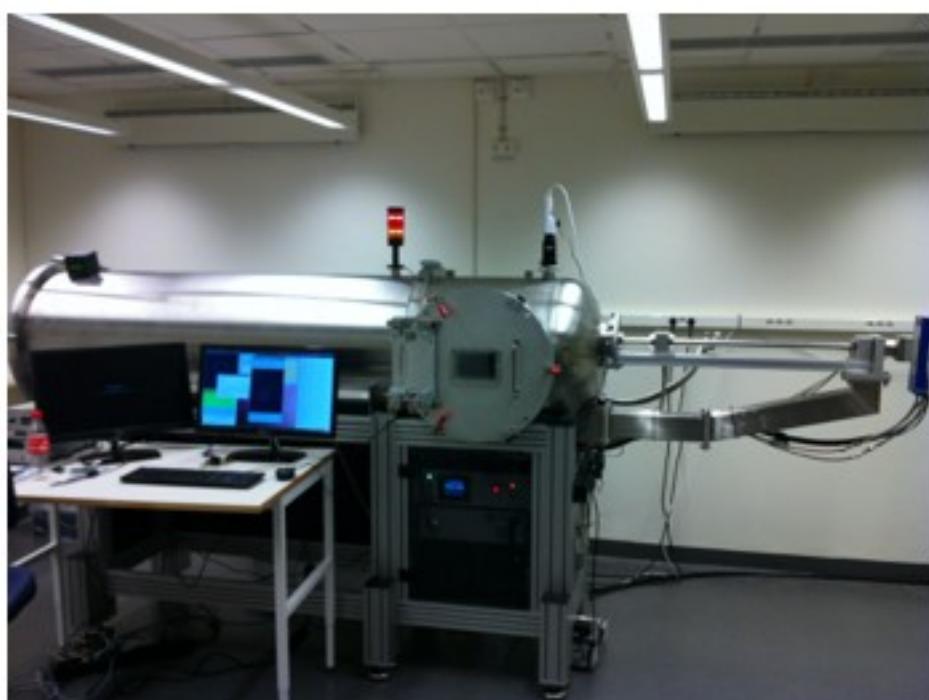
The **Small Angle X-ray Scattering (SAXS)** setup consists of:

- X-ray generator
- Göbel mirrors
- A three pin-hole collimation
- An integrated vacuum
- A 2D-gas detector

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SAXS: Laboratory pinhole camera



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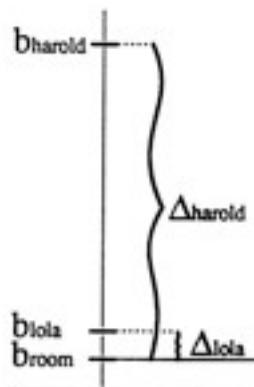
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5. Selected soft matter examples



Contrast and contrast variation

real life



When the master came, Lola like the peppered moth and the arctic hare, remained motionless and undetected. Harold, of course, was immediately devoured.



Excess scattering length density and contrast

$$\Delta\rho = \rho - \rho_{solv} = \frac{1}{V_1} \left(\sum_j b_j - \rho_{solv} V_1 \right)$$

basis for contrast variation

scattering amplitude of a discrete particle:

$$A(q) = \int_V d^3r e^{iq\cdot r} \Delta\rho(r)$$

position dependent excess scattering length density

Contrast variation: what determines $\Delta\rho$, how can we adjust $\Delta\rho$ for

Neutron

X-ray



SANS and scattering length

Scattering length difficult to calculate \rightarrow literature

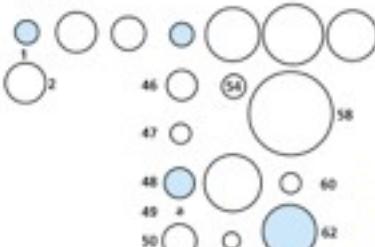
important findings:

- neutrons are scattered by nuclei
- weak interaction with matter \rightarrow large penetration depth \rightarrow ideal probe for optically dense materials
- depends on direction of nuclear spin \rightarrow magnetic scattering!
- b depends in an unsystematic way on the nucleus
- strong dependence on isotope used:

Contrast variation using isotopic substitution

H C O Ti Fe Ni U

Neutrons



SANS: Coherent vs. incoherent scattering

Differential cross section of an ensemble of scattering centers:

$$\frac{d\sigma}{d\Omega}(\vec{q}) = \sum_{j,k=1}^N \left\langle b_j b_k e^{i\vec{q} \cdot \vec{r}_{jk}} \right\rangle$$

b_j, b_k depend on isotope and spin state

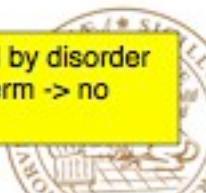
$$\begin{array}{ll} j \neq k: & \left\langle b_j b_k \right\rangle = \left\langle b_j \right\rangle \left\langle b_k \right\rangle = \langle b \rangle^2 \\ & \quad \quad \quad \nearrow \left\langle b_j b_k \right\rangle = \langle b \rangle^2 + \delta_{jk} (\langle b^2 \rangle - \langle b \rangle^2) \\ j = k: & \left\langle b_j b_k \right\rangle = \left\langle b_j^2 \right\rangle = \langle b^2 \rangle \quad \quad \quad \swarrow \end{array}$$

If spin state independent of position of scattering centers:

$$\frac{d\sigma}{d\Omega}(\vec{q}) = \langle b \rangle^2 \left[\sum_{j,k=1}^N \left\langle e^{i\vec{q} \cdot \vec{r}_{jk}} \right\rangle \right] + N(\langle b^2 \rangle - \langle b \rangle^2)$$

Coherent scattering: scattering from nuclei with the same average $\langle b \rangle$, contains structural information

Incoherent scattering: caused by disorder of isotopes, no interference term \rightarrow no structural information



SANS: Coherent vs. incoherent scattering

$$\frac{d\sigma}{d\Omega}(\vec{q}) = \langle b \rangle^2 \left[\sum_{j,k=1}^N \left\langle e^{i\vec{q} \cdot \vec{r}_{jk}} \right\rangle \right] + N(\langle b^2 \rangle - \langle b \rangle^2)$$

Coherent scattering:

- study collective properties of large number of scatterers

Typical example:

- spatial arrangements $\rightarrow S(q)$
- collective diffusion

Incoherent scattering:

- missing phase relation \rightarrow study behavior of individual scatterers

Typical example:

- Self diffusion

coherent and incoherent cross section:

$$\sigma_{coh} = 4\pi \langle b \rangle^2$$

$$\sigma_{incoh} = 4\pi (\langle b^2 \rangle - \langle b \rangle^2)$$



Neutron scattering cross section and scattering length

cross section values:

| isotope | nuclear spin | σ_{coh} in 10^{-28} m^2 | σ_{incoh} in 10^{-28} m^2 |
|-----------------|--------------|--|--|
| ^1H | 1/2 | 1.8 | 79.7 |
| ^2H | 1 | 5.6 | 2.0 |
| ^{12}C | 0 | 5.6 | - |
| ^{14}N | 1 | 11.6 | 0.3 |
| ^{16}O | 0 | 4.2 | - |

Coherent scattering length values:

| scattering length | ^1H | ^2H | ^{12}C | ^{16}O |
|-----------------------------|--------------|--------------|-----------------|-----------------|
| b in 10^{-14} m | -0.38 | 0.66 | 0.66 | 0.58 |

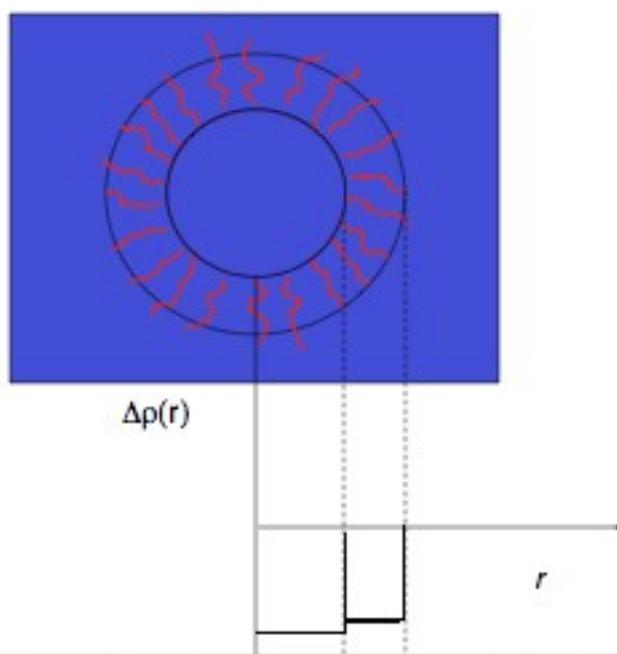
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SANS: Contrast variation

starting point:

| scattering length | ^1H | ^2H |
|-----------------------------|--------------|--------------|
| b in 10^{-14} m | -0.38 | 0.66 |



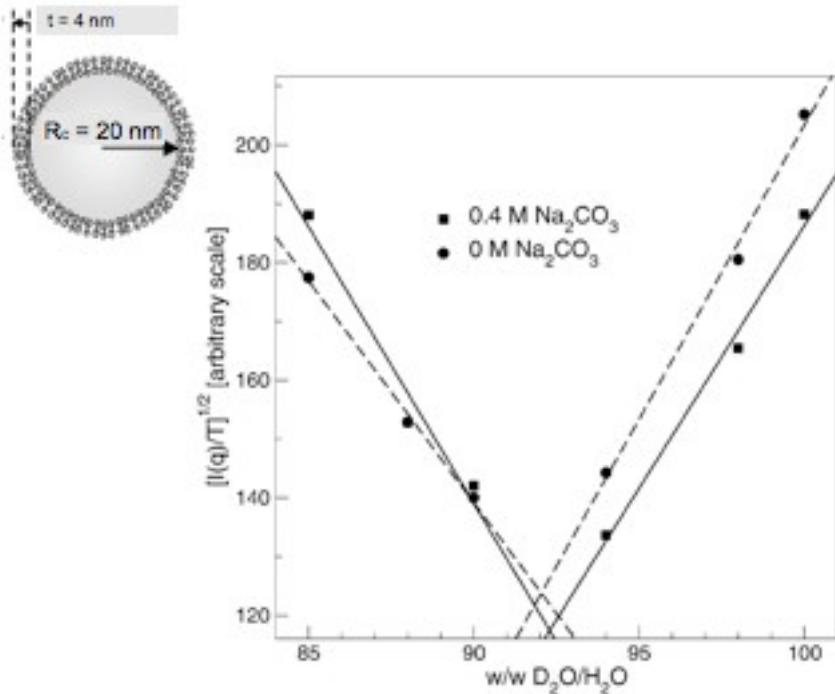
oil-in-water microemulsion

- h-oil and h-surfactant in D_2O
-> bulk contrast
- d-oil and h-surfactant in D_2O
-> shell contrast

Contrast variation allows to highlight individual parts of complex systems



Contrast variation study: Particles with d/h-PS core

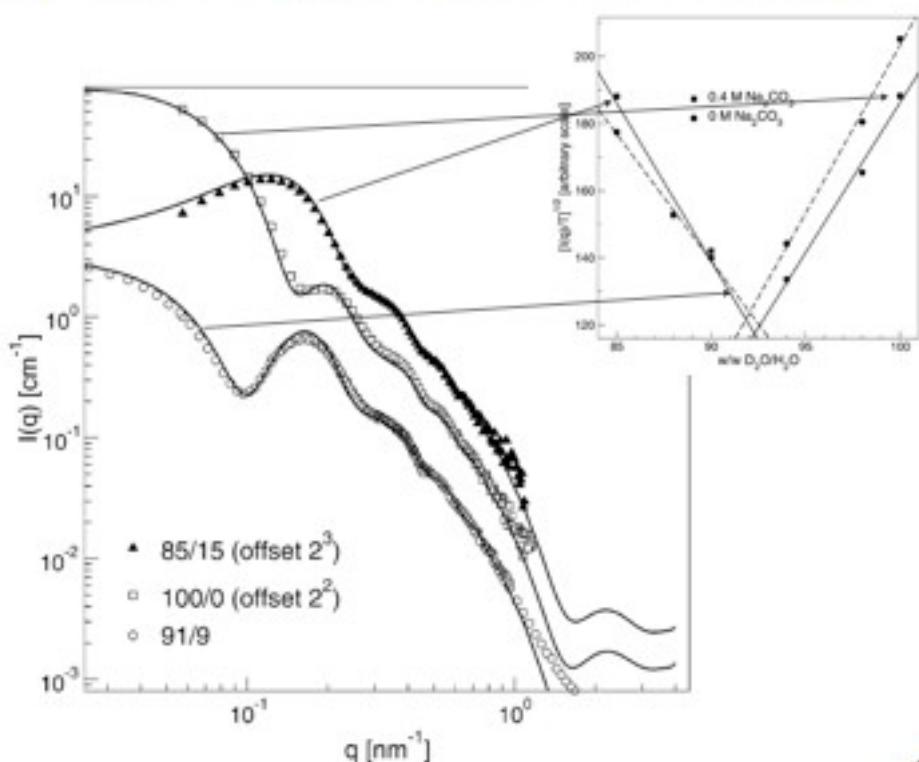


"Small-angle neutron scattering on a core-shell colloidal system: a contrast-variation study"
M. Zackrisson, A. Stradner, P. Schurtenberger, and J. Bergenholz, Langmuir 21, 10835-10845
(2005)

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Contrast variation study: Particles with d/h-PS core



"Small-angle neutron scattering on a core-shell colloidal system: a contrast-variation study"
M. Zackrisson, A. Stradner, P. Schurtenberger, and J. Bergenholz, Langmuir 21, 10835-10845
(2005)

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SANS contrast variation

Possible problems that can arise:

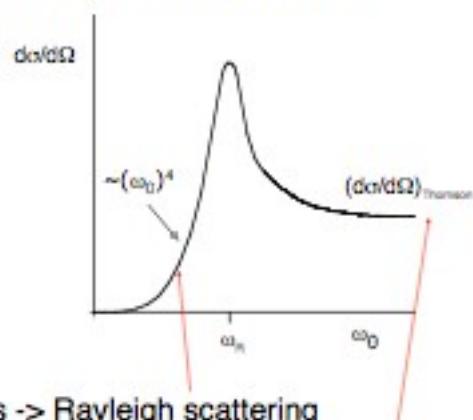
- **Change in solvent properties:** deuteration can shift the theta temperature for polymers or the location of a critical point. Example: shift of theta temperature of $\theta \pm 4$ °C for h-polystyrene in C₆D₁₂ or d-polystyrene in C₆H₁₂
- **Variation of melting point:** deuteration shifts the melting point for polymers. Example: $\Delta T \approx 6$ °C for polyethylene
- **Induces phase separation:** 50/50 mixture of h- and d-polystyrene phase separates in the melt
- **Shift in cmc:** the critical micellar concentration is generally higher in H₂O than in D₂O
- **Exchange of h and d:** Hydrogen or deuterium from certain groups (ex. OH or NH) can be exchanged -> overall excess scattering length density can vary with time, scattering length density of particles can be function of h/d ratio of solvent



SAXS and scattering length

Scattering of electromagnetic radiation is frequency dependent.

For a point scatterer we find:



- Visible light, low frequencies -> Rayleigh scattering
- $d\sigma/d\Omega$ peaks at resonance frequency ω_R
- For $\omega > \omega_R$: Thomson scattering for x-rays for single electron

Electron radius
 $r_{el} = e^2/m_e c^2$

$$\frac{d\sigma}{d\Omega} = r_{el}^2 \frac{1 + \cos^2 \theta}{2}$$

Scattering with unpolarized incident E-field



SAXS and scattering length

For scattering at small θ on electron cloud of an atom with Z number of electrons:

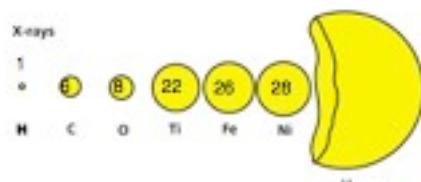
$$\frac{d\sigma}{d\Omega} = r_{el}^2 Z^2$$

contrast variation

In principle: Fourier transform of electron probability density

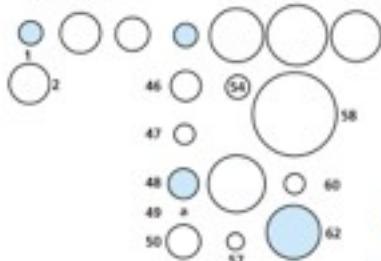
$$b = r_{el} Z$$

$$\Delta\rho = \rho - \rho_{solv} = r_{el} \left(\frac{\sum_j Z_j}{V_1} - \frac{\sum_k Z_{k,solv}}{V_1} \right)$$



H C O Ti Fe Ni U

Neutrons



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Summary: Scattering contrast for neutrons and X-rays

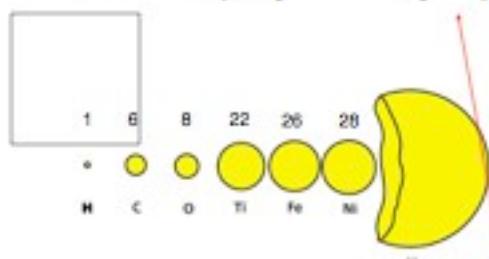
X-rays

scattering at small θ on electron cloud of an atom with Z number of electrons:

$$\frac{d\sigma}{d\Omega} = r_{el}^2 Z^2$$

Fourier transform of electron probability density

$$\Delta\rho = \rho - \rho_{solv} = r_{el} \left(\frac{\sum_j Z_j}{V_1} - \frac{\sum_k Z_{k,solv}}{V_1} \right)$$



contrast variation

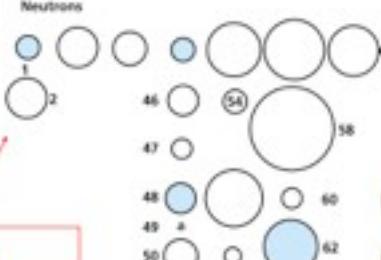
Neutrons

Scattering length from QM \rightarrow literature

- neutrons scattered by nuclei
- weak interaction with matter \rightarrow large penetration depth
- depends on direction of nuclear spin \rightarrow magnetic scattering!
- b depends in an unsystematic way on the nucleus
- strong dependence on isotope used:

H C O Ti Fe Ni U

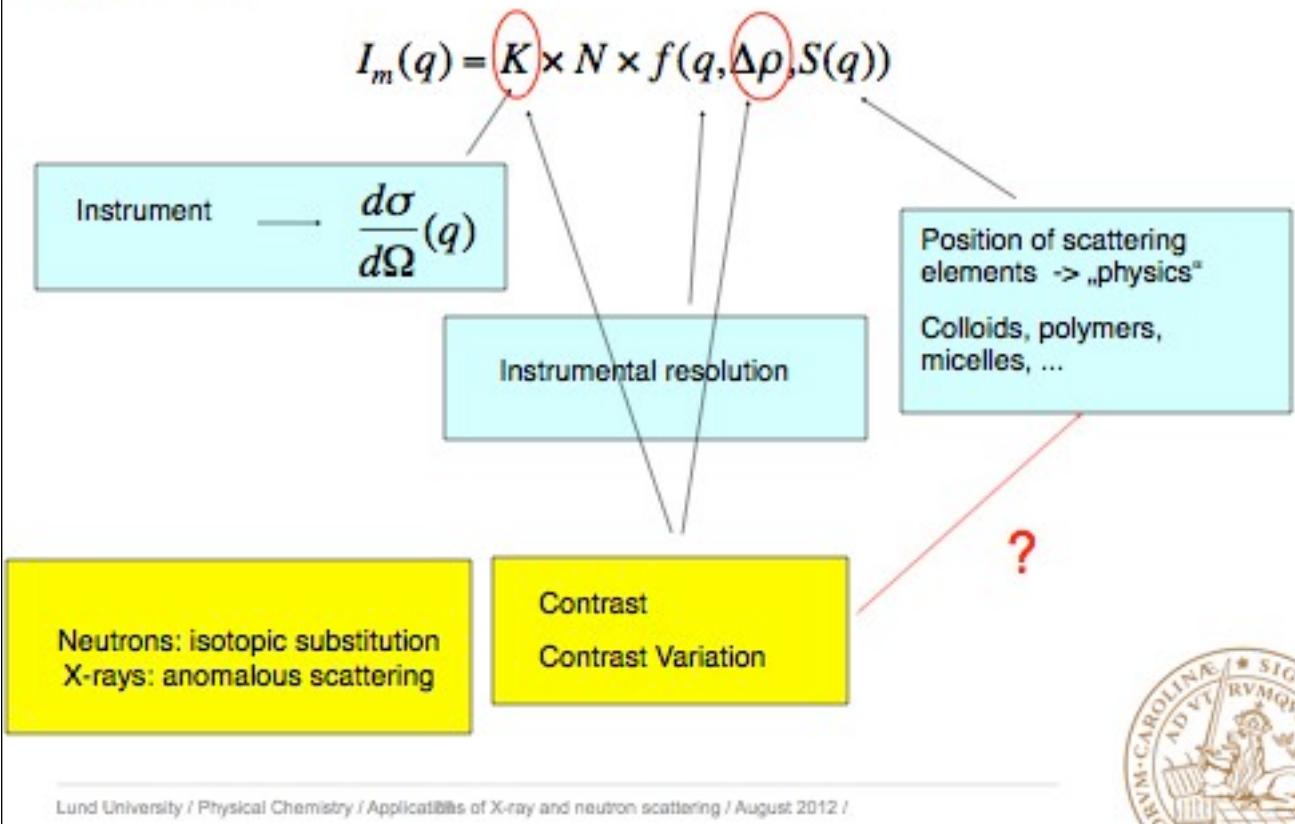
Neutrons



Lund University / P

Summary

A small-angle scattering experiment (SANS, SAXS): Ensemble of N identical particles - What do we really measure?



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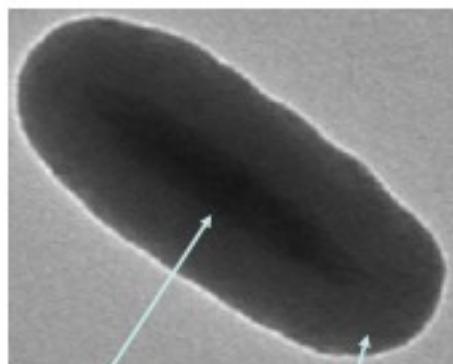
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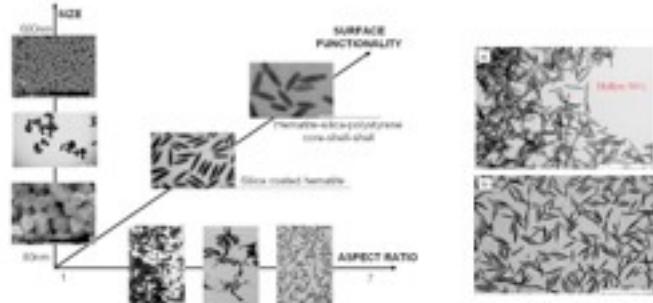


1st example: magnetic nanoparticles

hematite through forced hydrolysis of iron salts, coated with SiO_2 shell



Non-centrosymmetric hard and soft potential



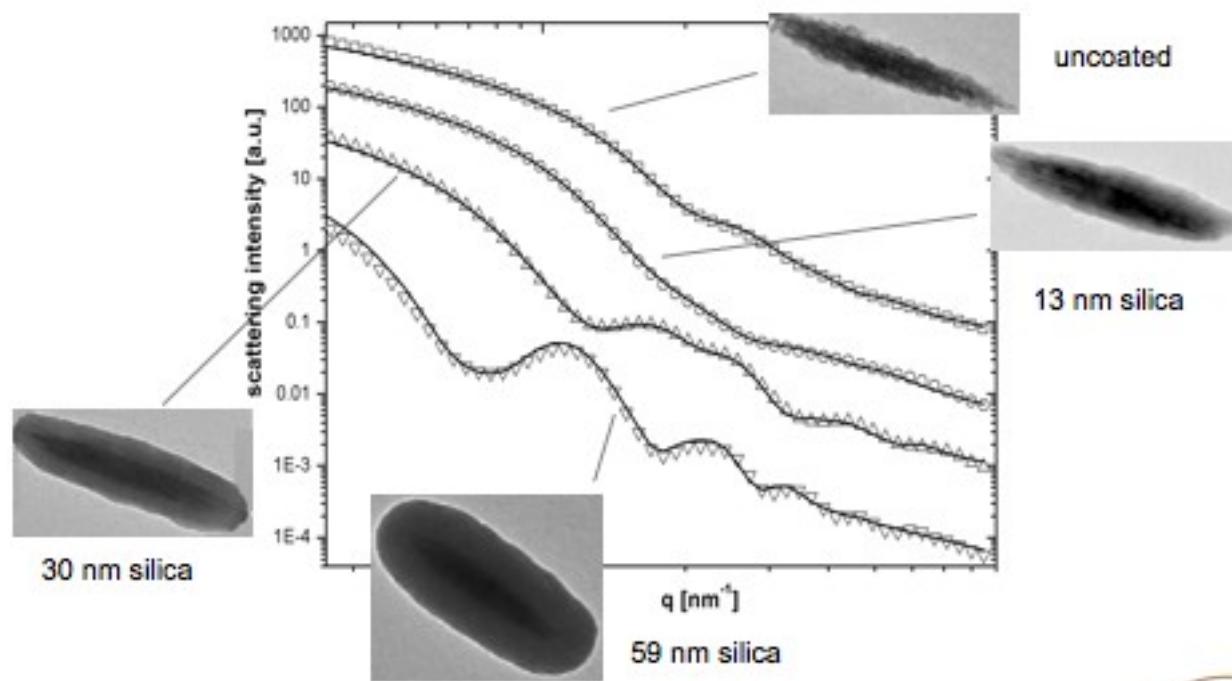
hematite core,
aspect ratio 1 to 7

SiO_2 shell,
with thickness 10 to 60 nm

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Structural information from SAXS



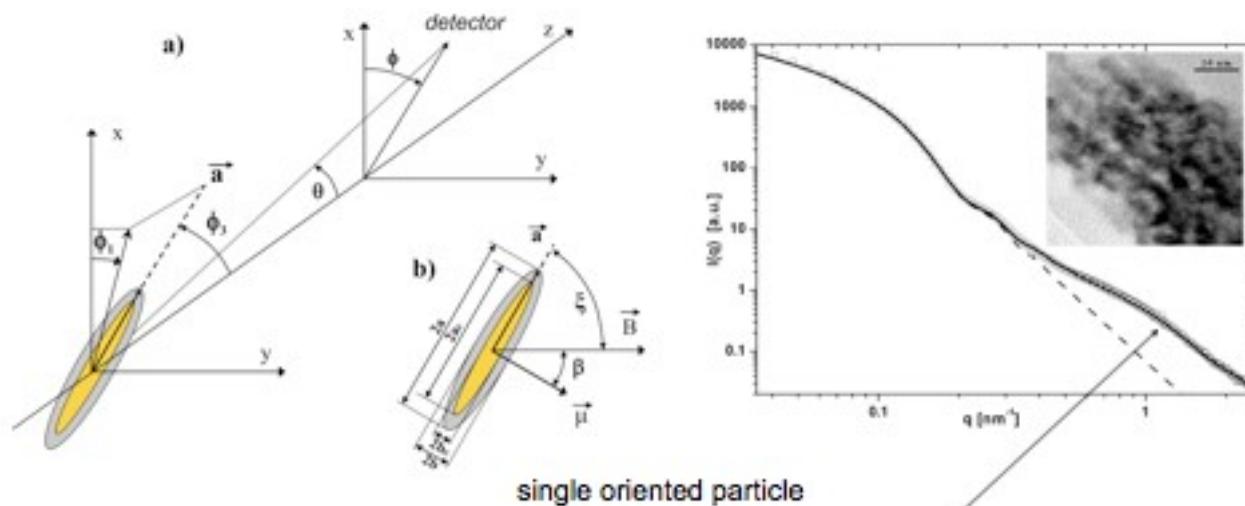
M. Reufer et al, J. Phys. Chem. B (2010)

M. Reufer et al, J. Phys. Cond. Mat. (2011)

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SAXS modeling: size, anisotropy, structure, porosity

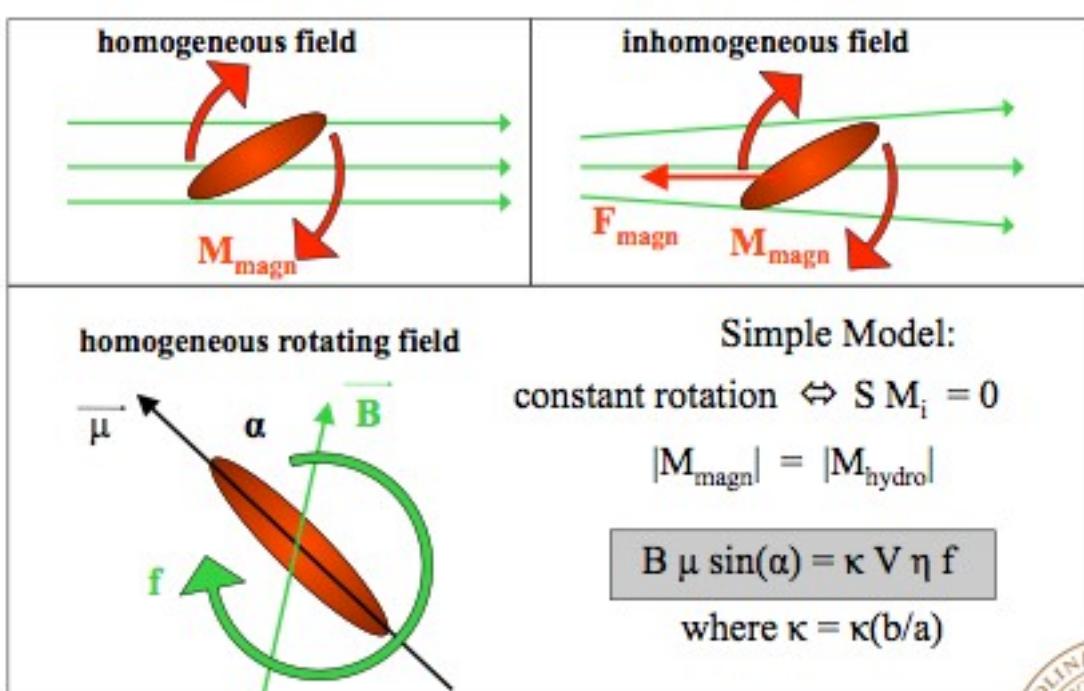


$$I^{\text{iso}}(q) = \int_0^{2\pi} \int_0^\pi \left[F_{\text{core-shell-ellipse}}^2(\phi_1, \phi_3) + N_{\text{pores}} F_{\text{pore}}^2 \right] \sin(\phi_3) d\phi_1 d\phi_3$$

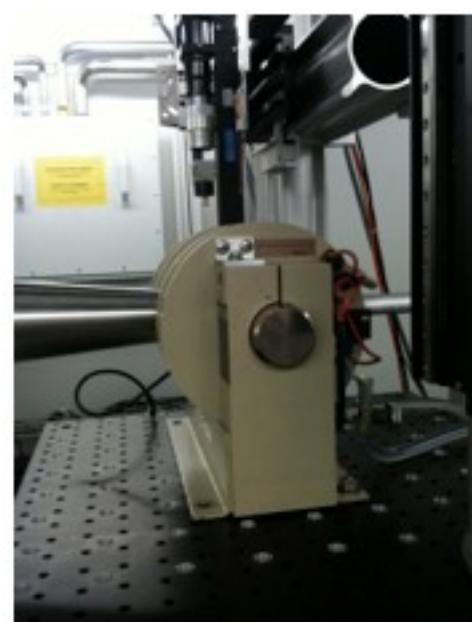
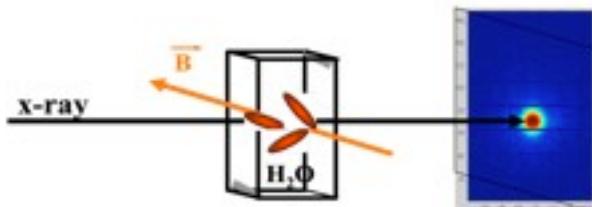
=> size, coating thickness, polydispersity, porosity



Magnetic particles in a magnetic field



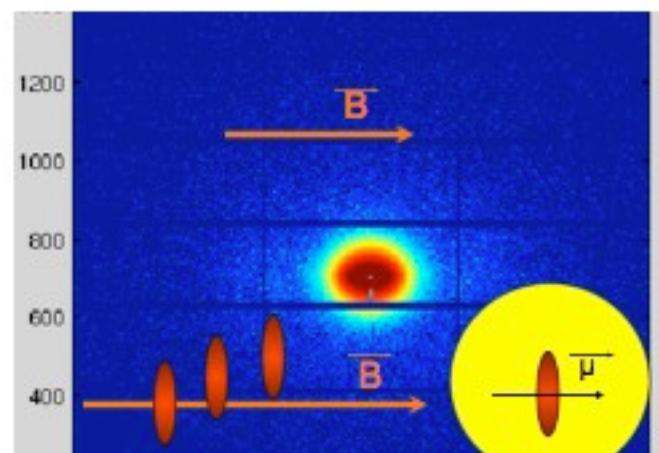
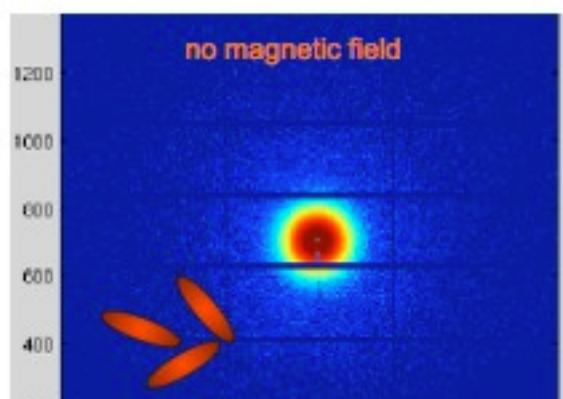
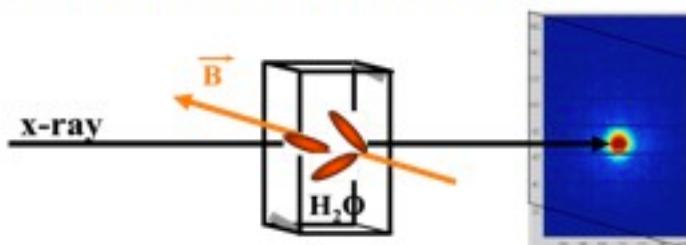
SAXS with an applied magnetic field



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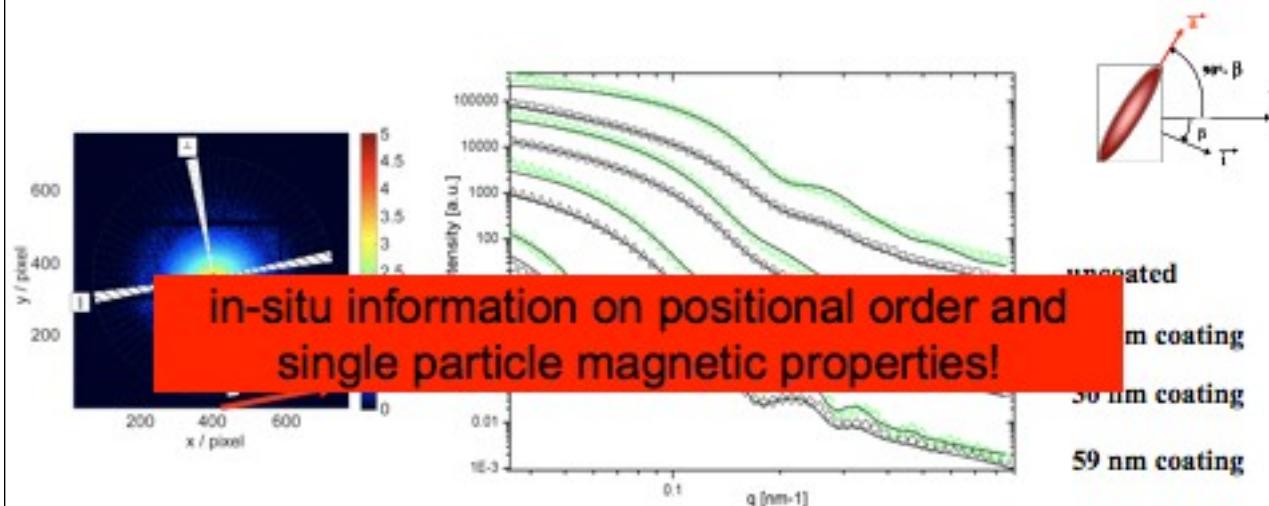
SAXS with an external magnetic field



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SAXS with an applied magnetic field



in-situ information on positional order and single particle magnetic properties!

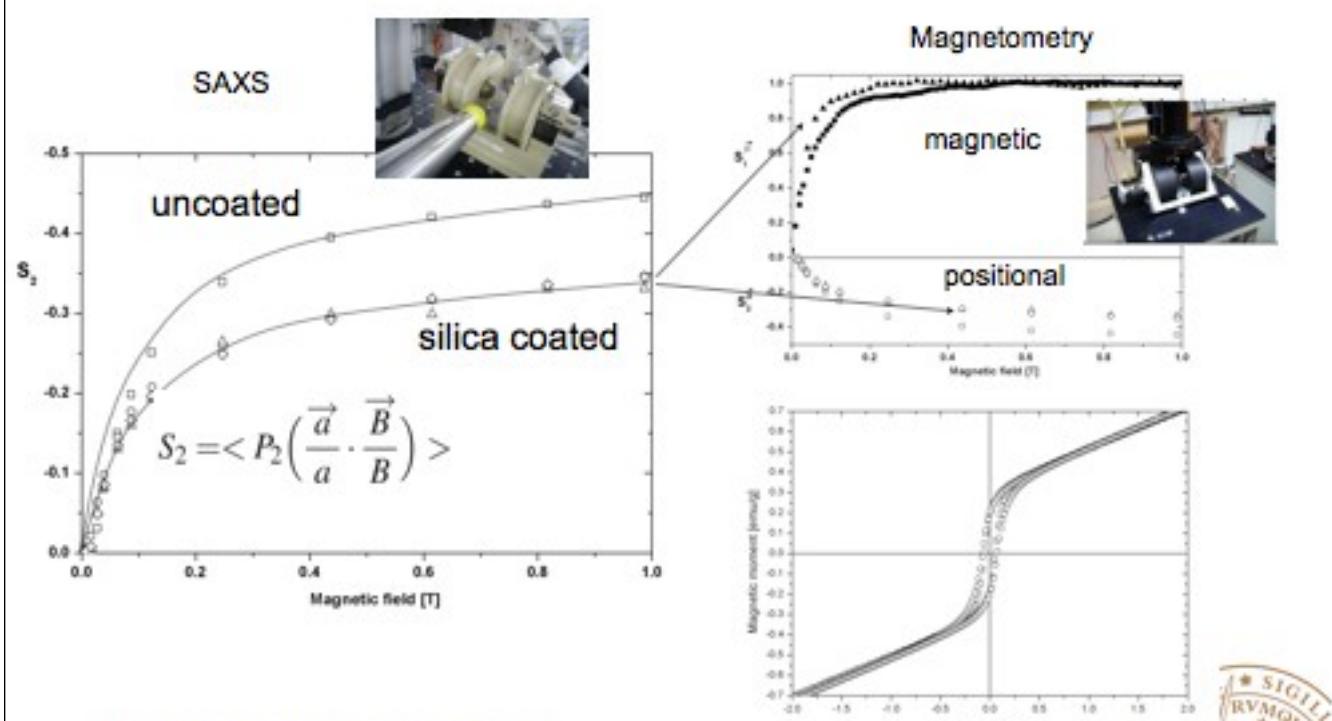
$$P(q, \phi, a, b, a_c, b_c) = \frac{1}{Z} \int_0^{2\pi} \int_0^\pi p(E_{\text{pot}}) \left\{ [\tilde{\rho}_R R(a, b) + \tilde{\rho}_c R(a_c, b_c)]^2 + \sum_m N_{pm} [\tilde{\rho}_p R(a_{pm}, b_{pm})]^2 \right\} \sin(\phi_3) d\phi_1 d\phi_3$$

M. Reufer et al, J. Phys. Chem. B (2010)

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Orientational and magnetic order parameter



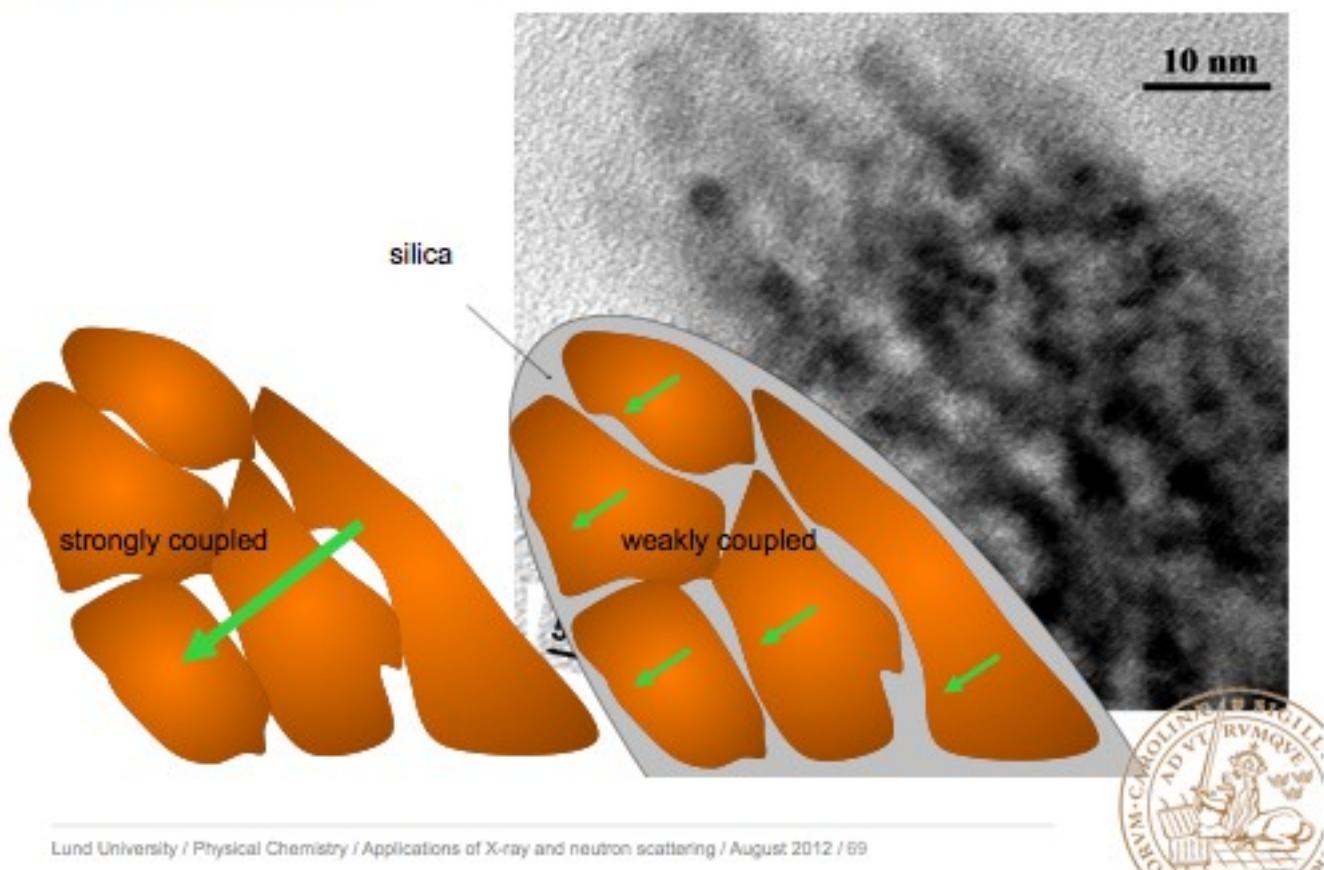
M. Reufer et al, J. Phys. Chem. B (2010)

M. Reufer et al, J. Phys. Cond. Mat. (2011)

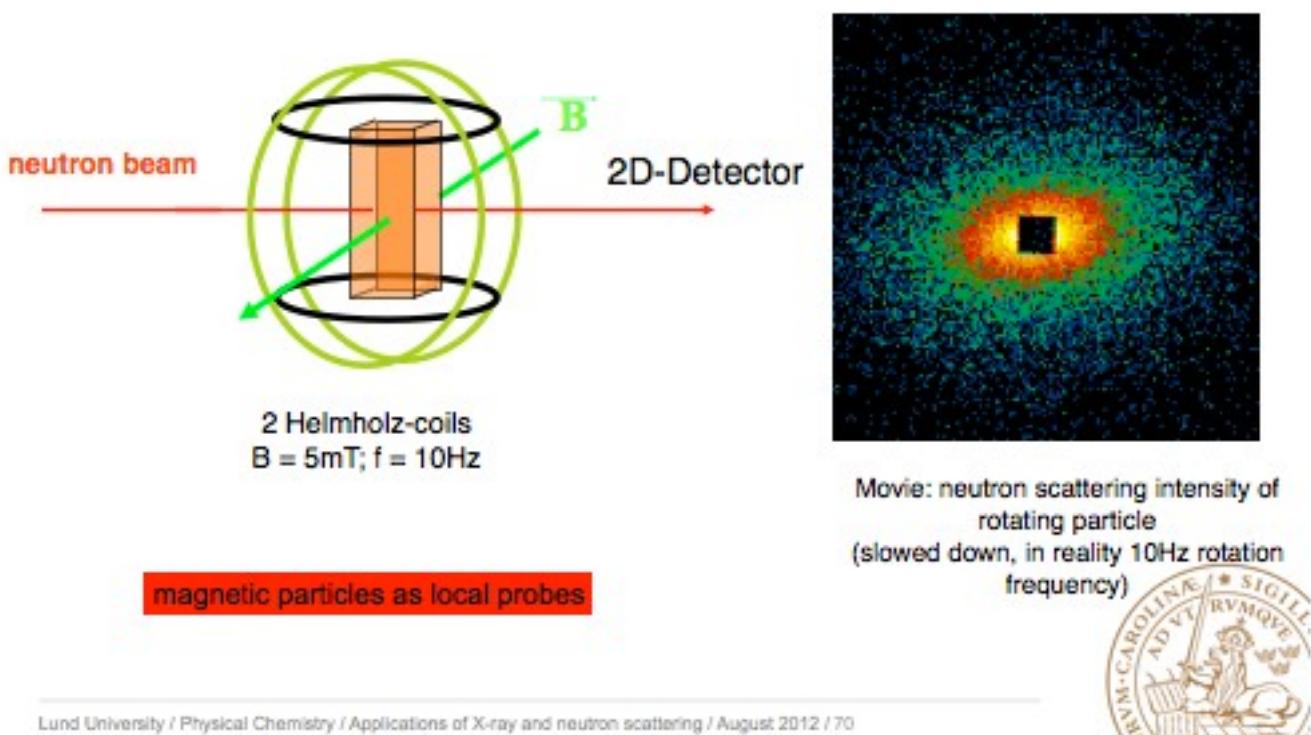
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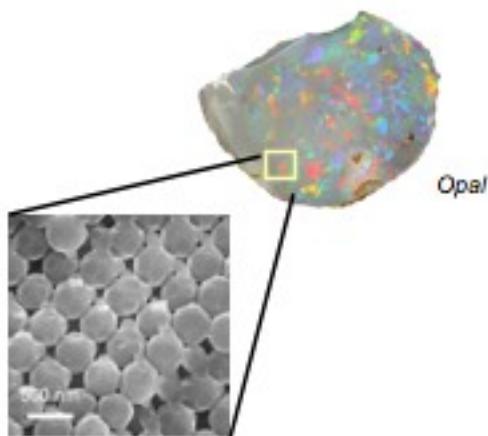
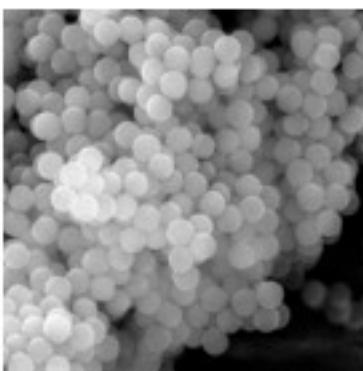
critical size for hematite: ~ 30 nm



Stroboscopic SANS or SAXS



2nd example: hard sphere systems

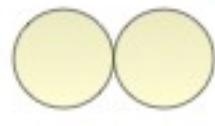
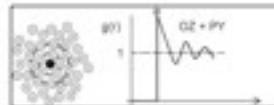


Insight from SANS

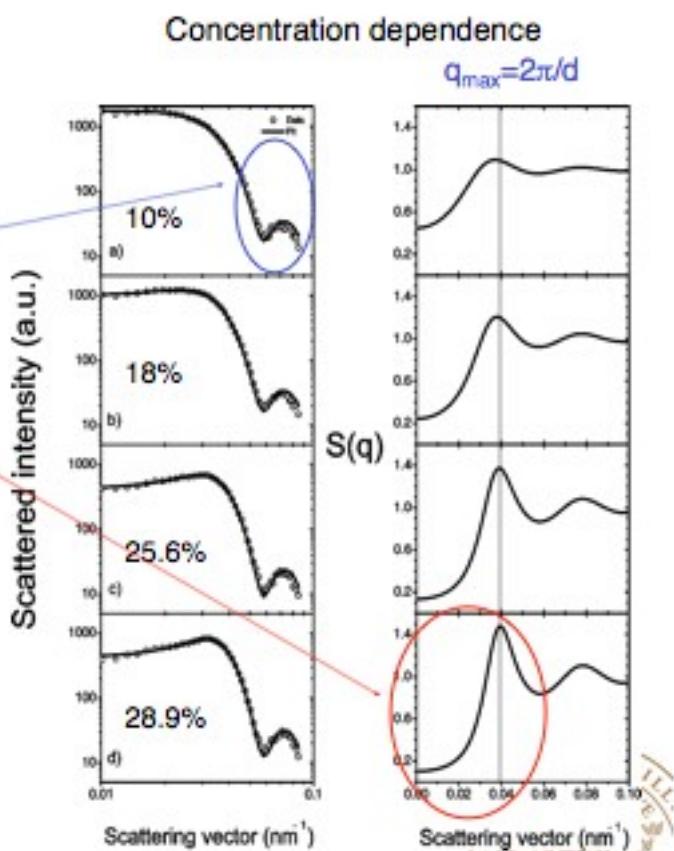
Scattering intensity: contributions from particle size and interparticle correlations

$$I(q) = P(q)S(q)$$

Hard sphere suspensions:

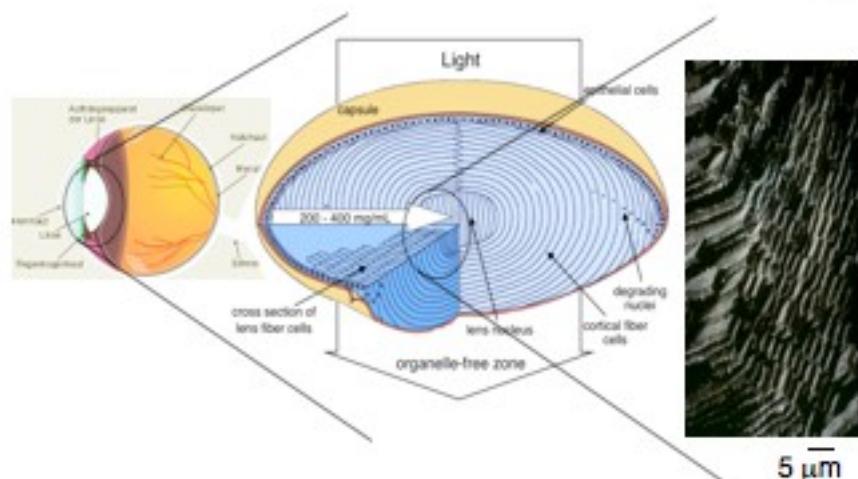


Colloidal suspensions ($a=85\text{ nm}$
Polystyrene spheres in $\text{H}_2\text{O}/\text{D}_2\text{O}$)



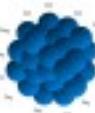
An application: Why is the eye lens transparent?

The fiber cells consist of a highly concentrated protein solution:



Alpha-crystallins:

~ 800 kDa
specific volume:
~ 1.5 - 1.7 mL/g



Beta-crystallins:

$\beta_H \sim 200$ kDa;
 $\beta_L \sim 50$ kDa



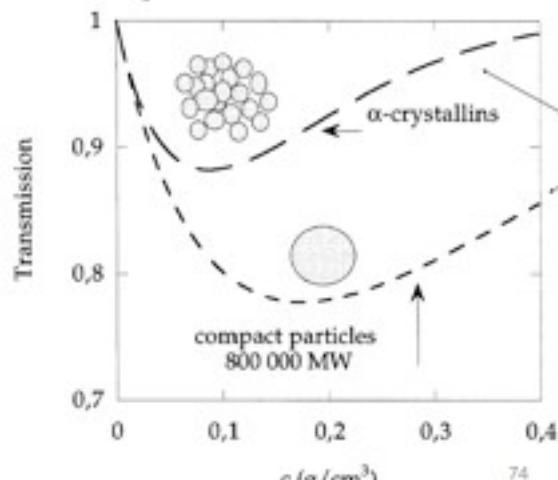
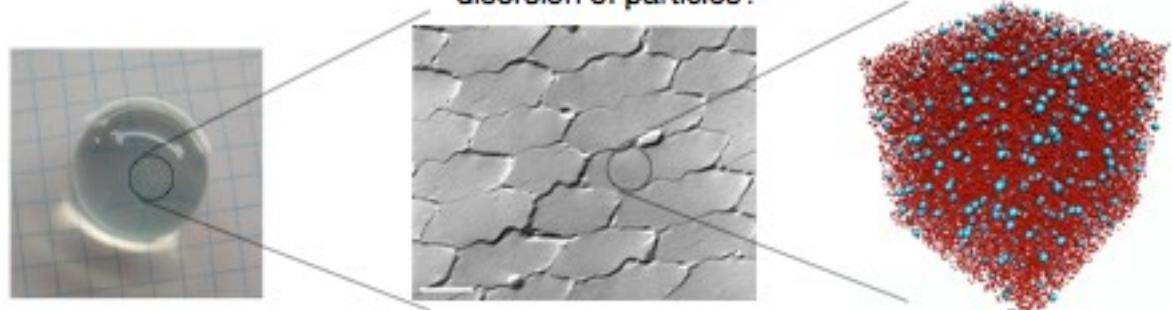
Gamma-crystallins:

~ 20 kDa
specific volume:
~ 0.7 mL/g



An application: Why is the eye lens transparent?

Why is the eye lens transparent despite the fact that it contains a highly concentrated dispersion of particles?

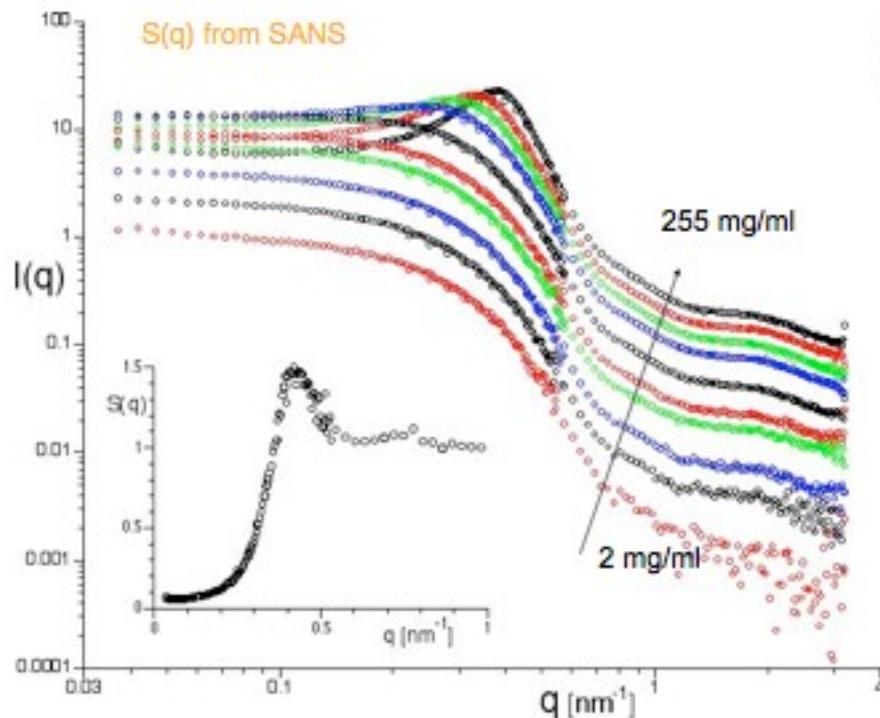


Transmission from intensity at all scattering vectors with

$$I(q) = P(q)S(q)$$



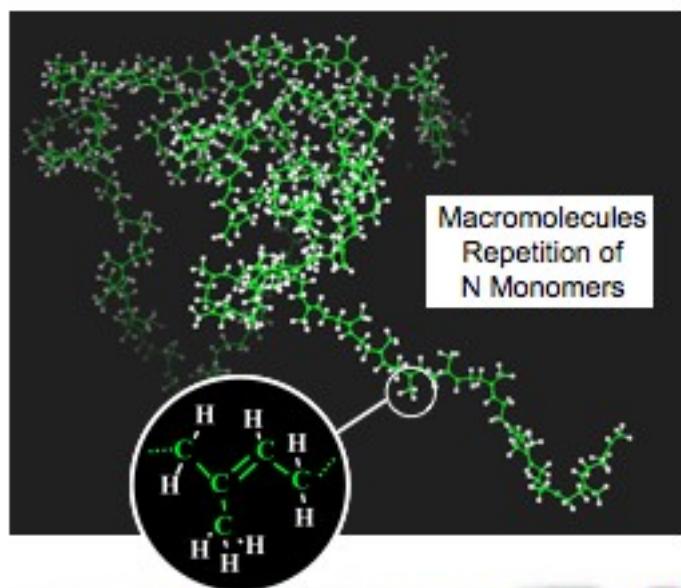
α -crystallins as model hard spheres?



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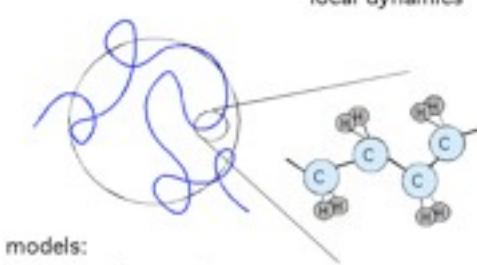


Scattering and soft matter - selected examples



global properties: radius

local properties:
local dynamics

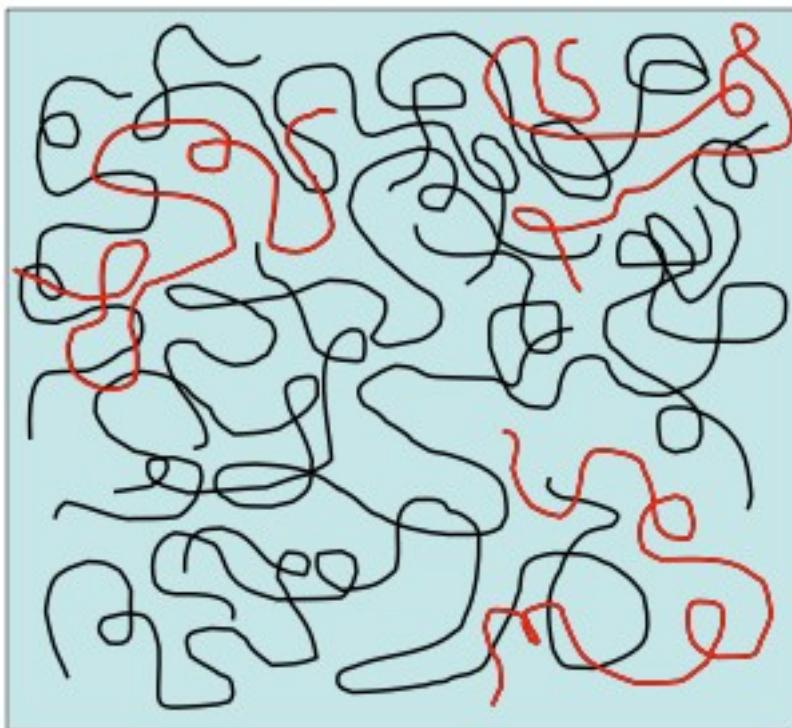


molecular dynamics
simulations



How does a polymer look in the melt or the essence of contrast variation

polymer melt



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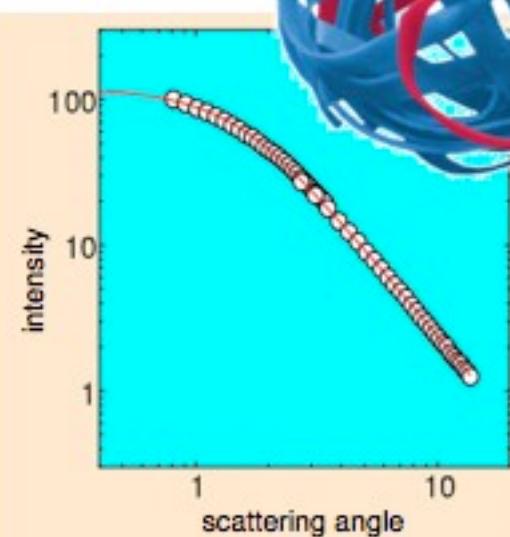
Polymer conformation in the melt?



P.J. Flory
Stanford
USA

Nobel prize 1974

Kirste et al.
Jülich 1974

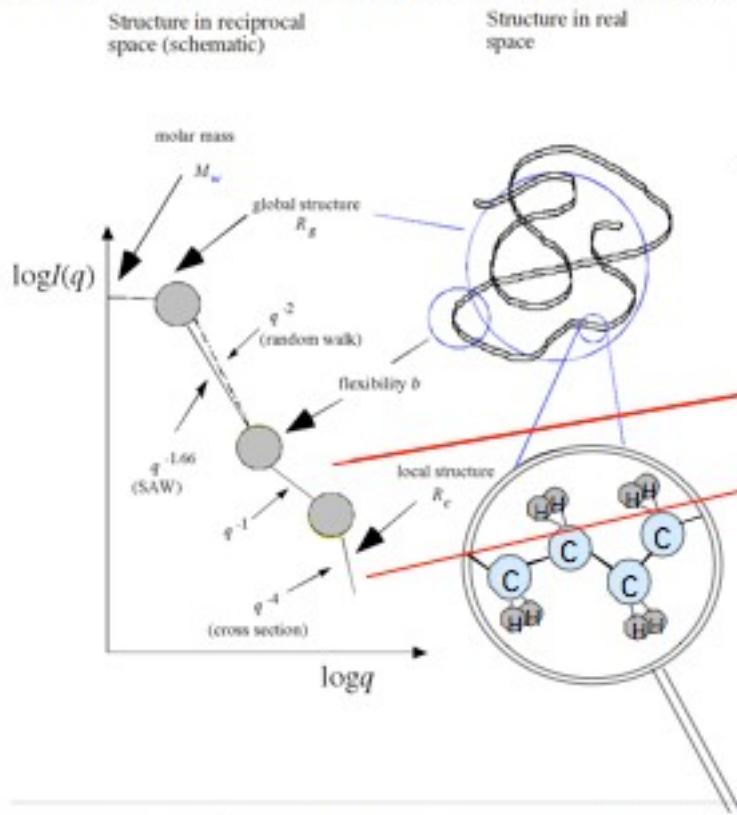


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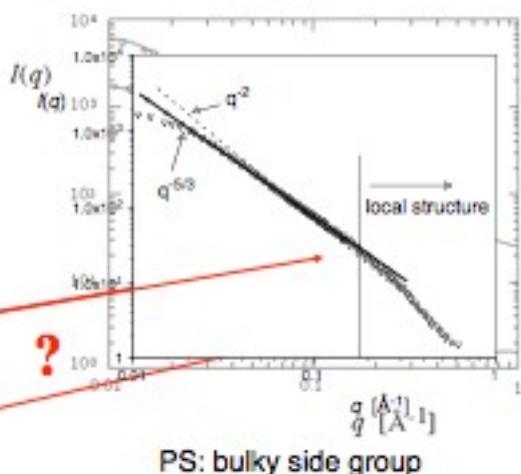


Selected SANS examples: Polymer conformation

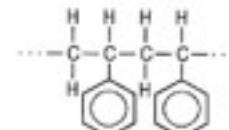
Schematic q-dependence of polymer chain in dilute solution:



Experiment with polystyrene:



PS: bulky side group



Rawiso et al., 1980

