

Fundamentals of small angle neutron scattering (SANS)

Shibayama, & CROSS

3rd day (Aug. 12)
9:00 - 10:30

Mitsuhiro Shibayama

**Comprehensive Research Organization for
Science and Society (CROSS), Japan**

**<https://neutron.cross.or.jp/mitsu/>
<https://neutrons.cross.or.jp/en/>**

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CUHK Lecture, M. Shibayama
2025.8.10 - 16

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2. SANS instruments
3. Angle dispersion vs TOF measurements

Part 2. Basics of Neutron scattering

Part 3. SANS theory

1. Guinier law
2. Form factors (sphere, cylinder, etc.)
3. Porod law
4. Polymer
5. Interacting systems
6. One-phase systems (Ornstein-Zernike)
7. Multi-phase systems (Debye-Bueche)
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8. Asymptotic behaviors

Part 4. Analysis

1. Q-space analysis
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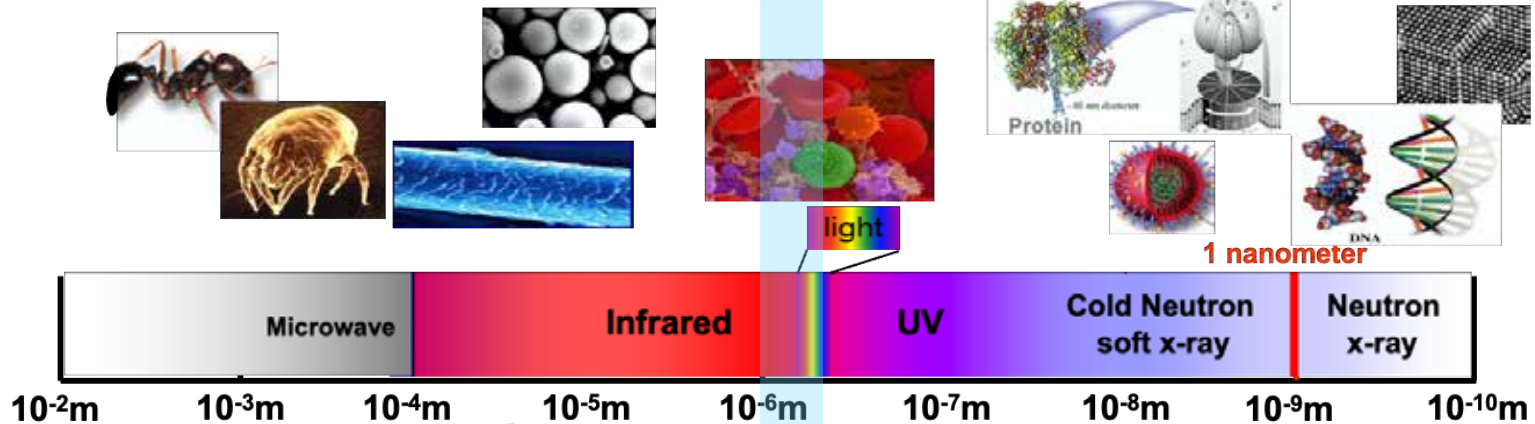
Part 6. Summary and reference

Materials science

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Natural

Optical limit of
light
~ 250nm



Ernst Karl Abbe
19C (1873)

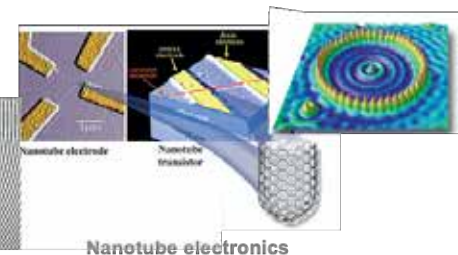
Manmade

We need

Electron Microscopy (destructive)
STM (surface)
In-situ analysis : Neutron & X-ray



Antonie van Leeuwenhoek
17C



From lab instruments to large facilities

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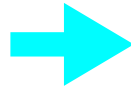
Laboratory



Microscope

Optical microscope

Seeking
Better resolution,
Larger flux,
Higher brilliance, ...



Electron microscope



AFM



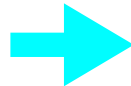
Cryo-TEM

Large facilities

X-ray



Lab X-ray



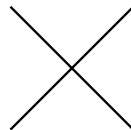
Shanghai Synchrotron
Radiation Facility
(SSRF)



SPring-8, JP

synchrotron X-ray

Neutron



China Spallation
Neutron Source CSNS

5

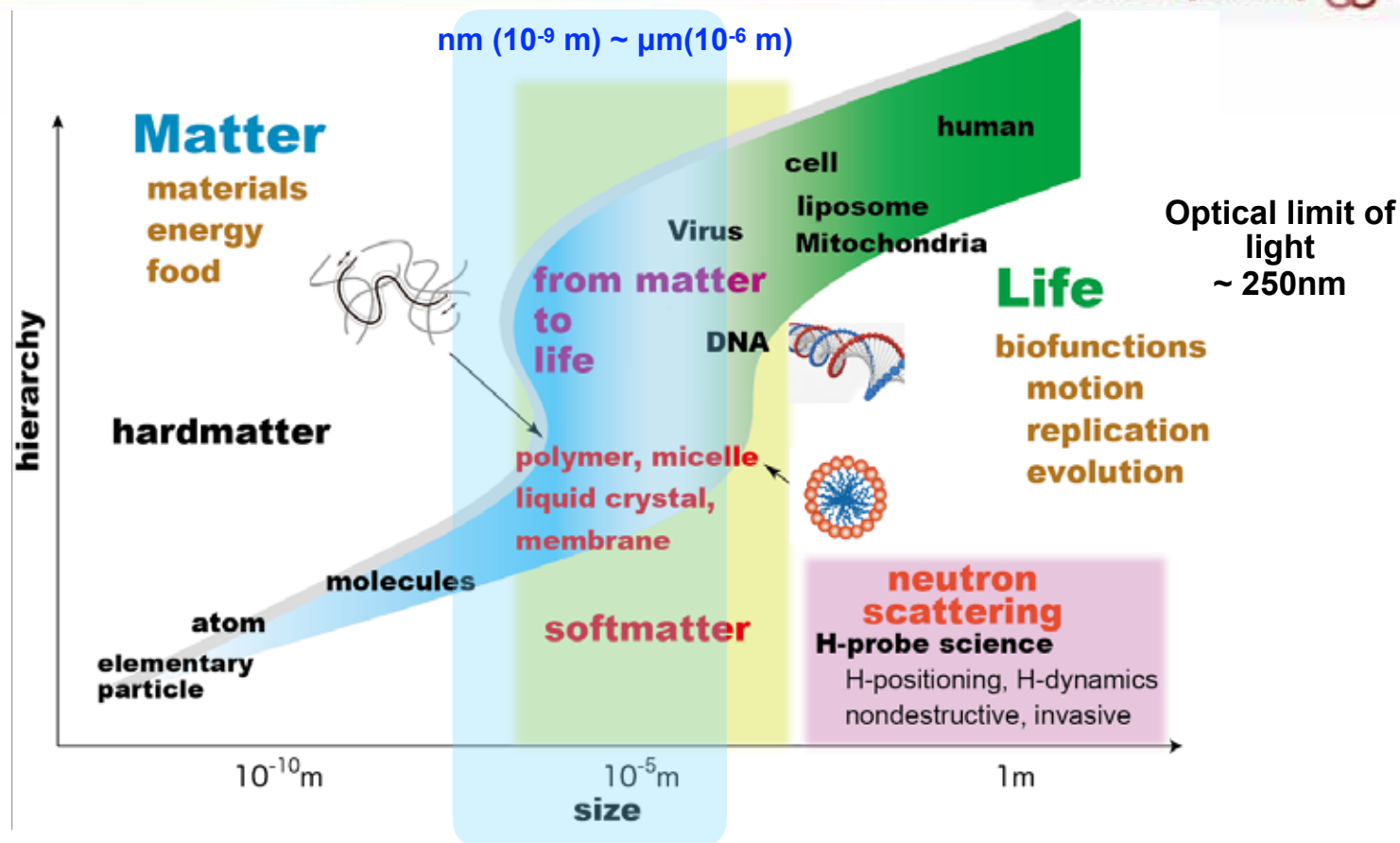


J-PARC, JP

Neutron

Size-hierarchy relationship of matter

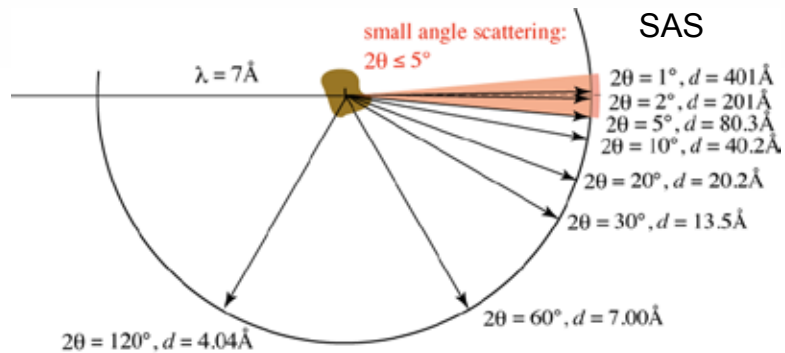
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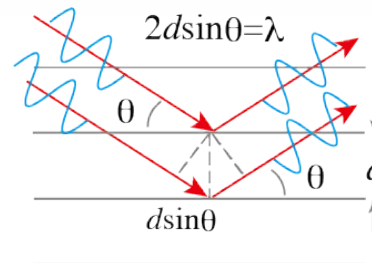
Important range in size and hierarchy contributing to properties/functions of matter, etc.

Small angle scattering (SAS): overview

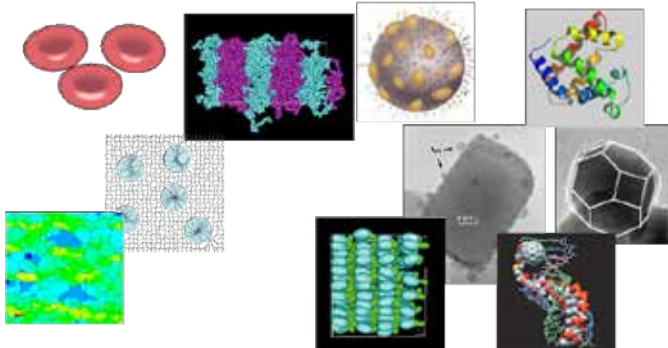
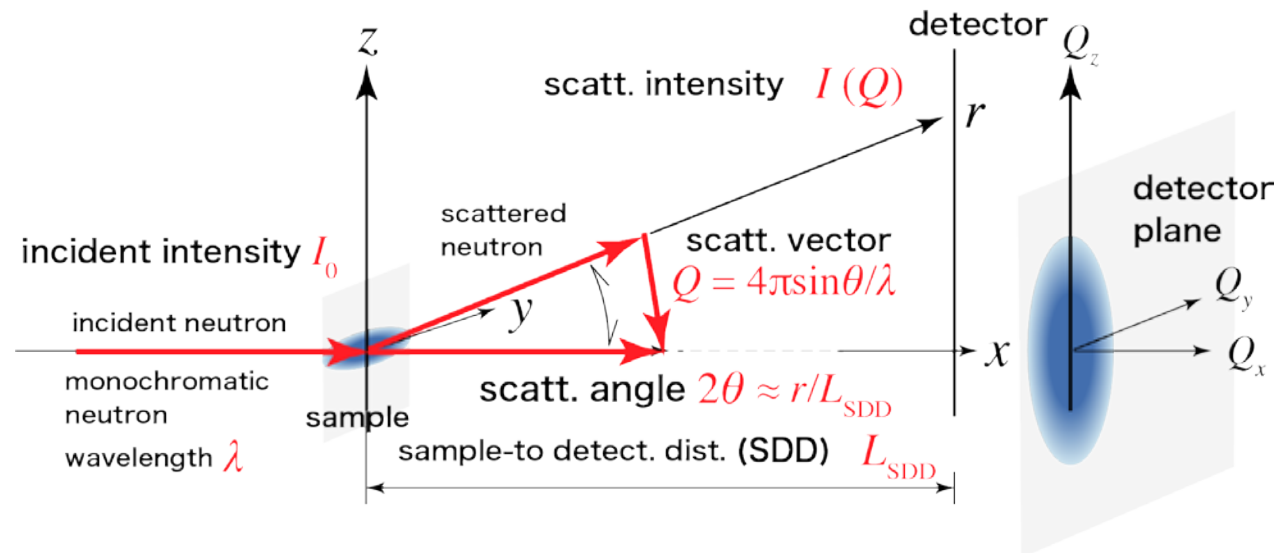
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Bragg's law : $2d \sin \theta = \lambda$



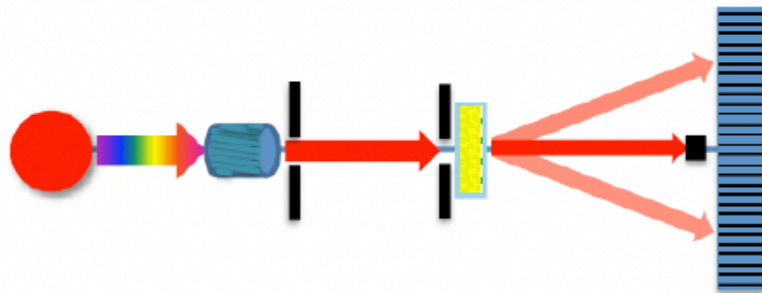
SAS



Reactor source vs pulse source

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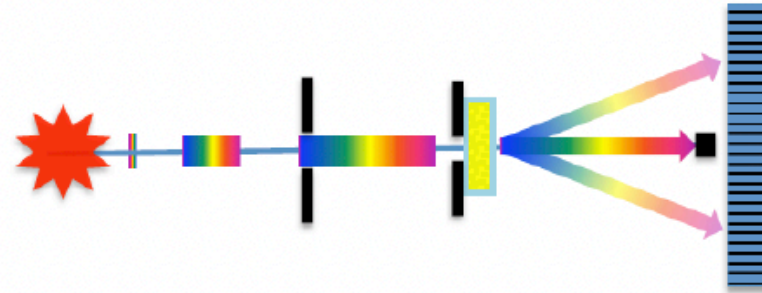
Continuous Reactor source



Monochromatic - narrow spectral band

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

Pulsed Spallation



TOF – wide spectral band

$$Q = 4\pi\sin\theta / \lambda[D, \text{TOF}]$$

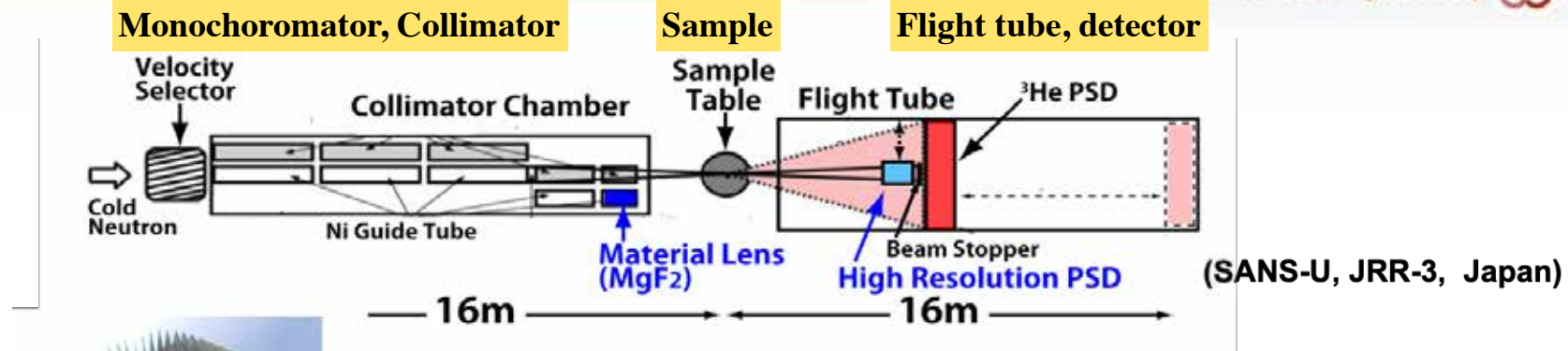
Courtesy of of E. Gilbert, Neutron and Muon School, Tokai, 2021

SANS instrument (SANS-U, ISSP)

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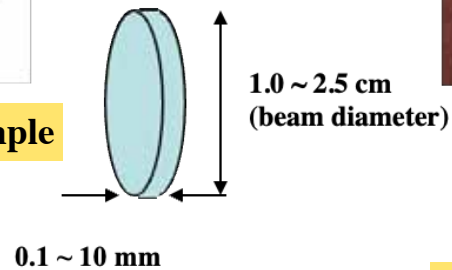
Okabe, et al., Nuclear Inst. and Methods in Physics Research, A, 2007, 572, 853.

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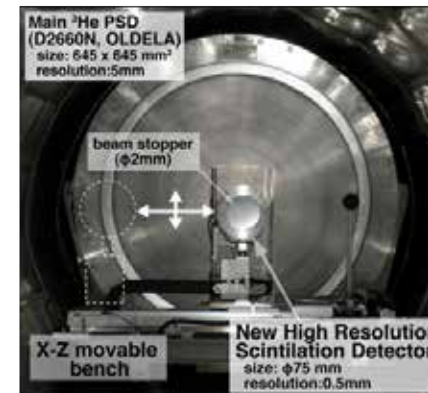


Typical sample size

Sample



Sample holder



J. Appl. Crystallogr., 2011, 44, 558.

- SANS is used for structural investigation for solid, liquid, polymers, etc., of the order of **1 nm – 100 nm**.

BL15 TAIKAN

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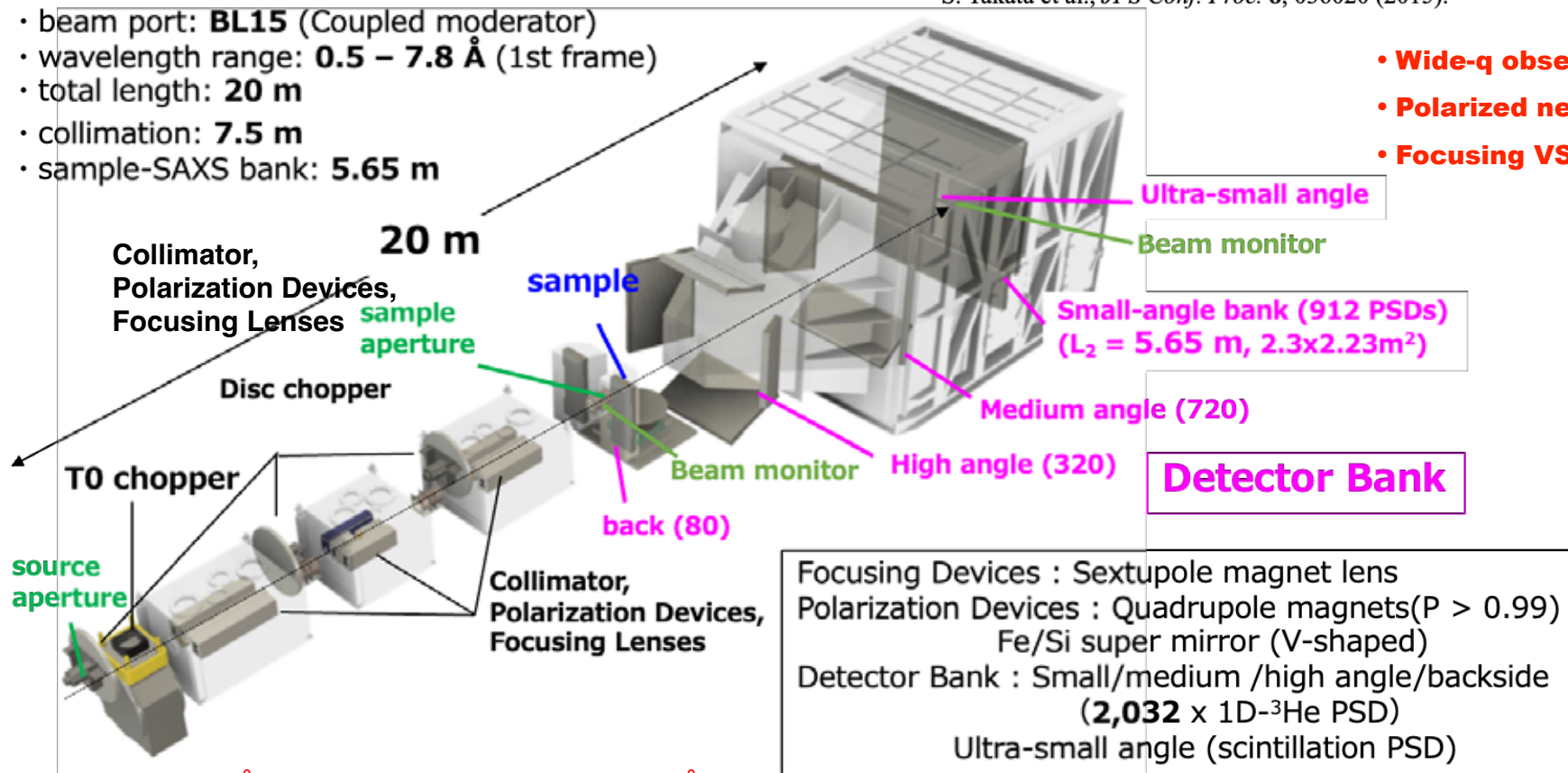
Small and Wide Angle Neutron Scattering Instrument

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Time-of-Flight Small and Wide angle Neutron Scattering Instrument

S. Takata et al., JPS Conf. Proc. 8, 036020 (2015).

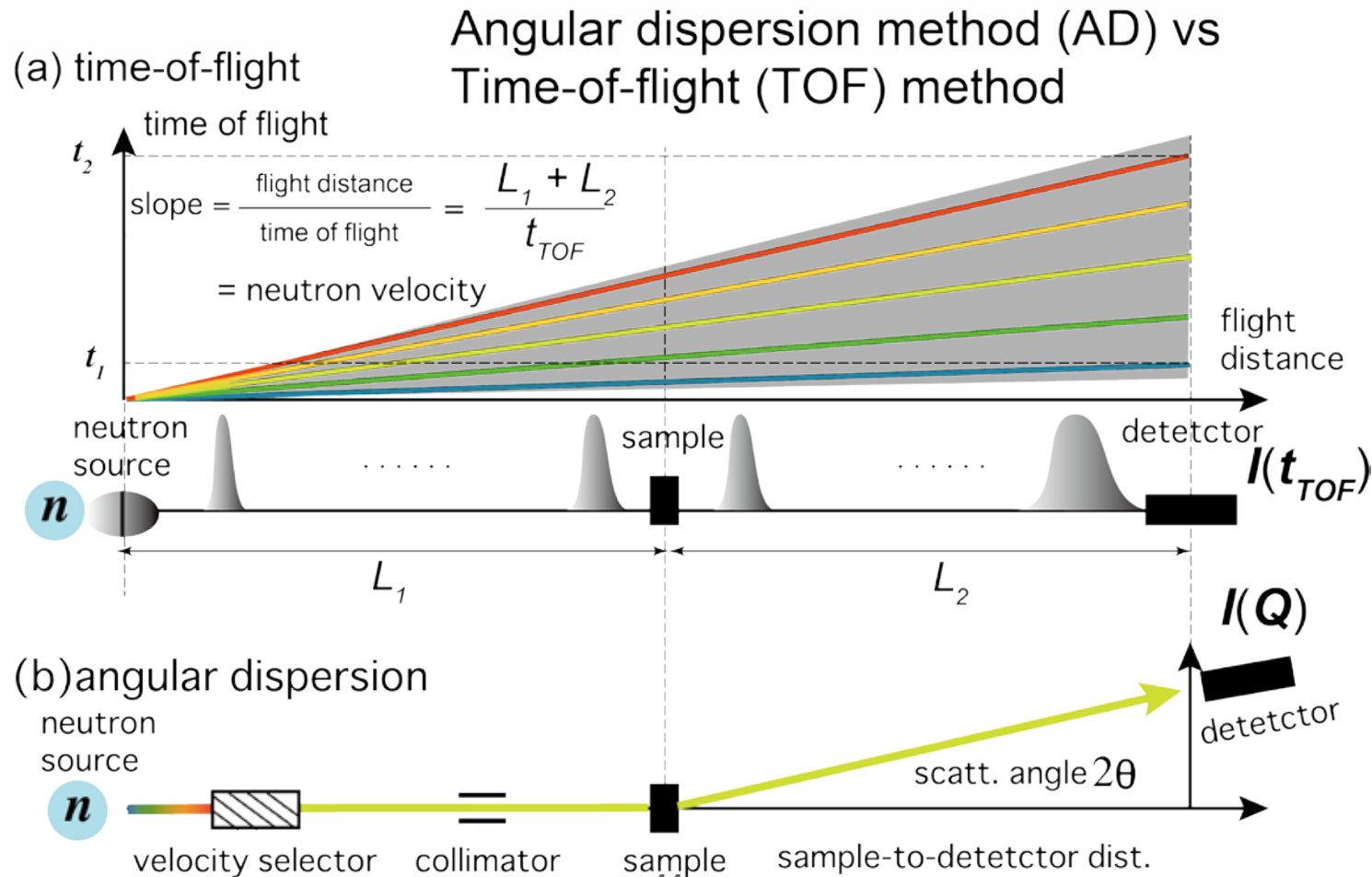
- beam port: **BL15** (Coupled moderator)
- wavelength range: **0.5 – 7.8 Å** (1st frame)
- total length: **20 m**
- collimation: **7.5 m**
- sample-SAXS bank: **5.65 m**



Q-range: $5 \times 10^{-3} - 17 \text{ Å}^{-1}$ (optionally, $Q_{\min} = 8 \times 10^{-4} \text{ Å}^{-1}$)

TOF vs AD methods

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CSNS,
J-PARC MLF
ISIS,
SNS
...

JRR-3,
ANSTO
ILL
ORNL
NIST
...

Initial planning; experimental design

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(1) What kind of information do I want to obtain?

Particle size, long spacing, interfacial thickness, correlation length,
Inter-particle potential, ...

(2) What kind of sample(s) do I want to measure?

Solid (film, powder, ..), liquid (micelle, polymer solution, gel, ..), gas

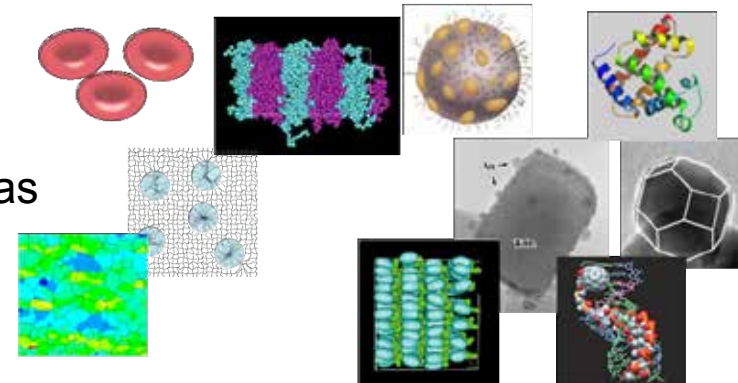
(3) Is it accessible with SANS?

Length scale: $\sim 10\text{\AA}$ - $\sim 1000\text{\AA}$

Sample size: cm large, mm thick

Neutron Scattering contrast: calculation of SLDs

Sample environment: Temp., Pressure,
Stress (strain), shear, flow, Mag. Field,...



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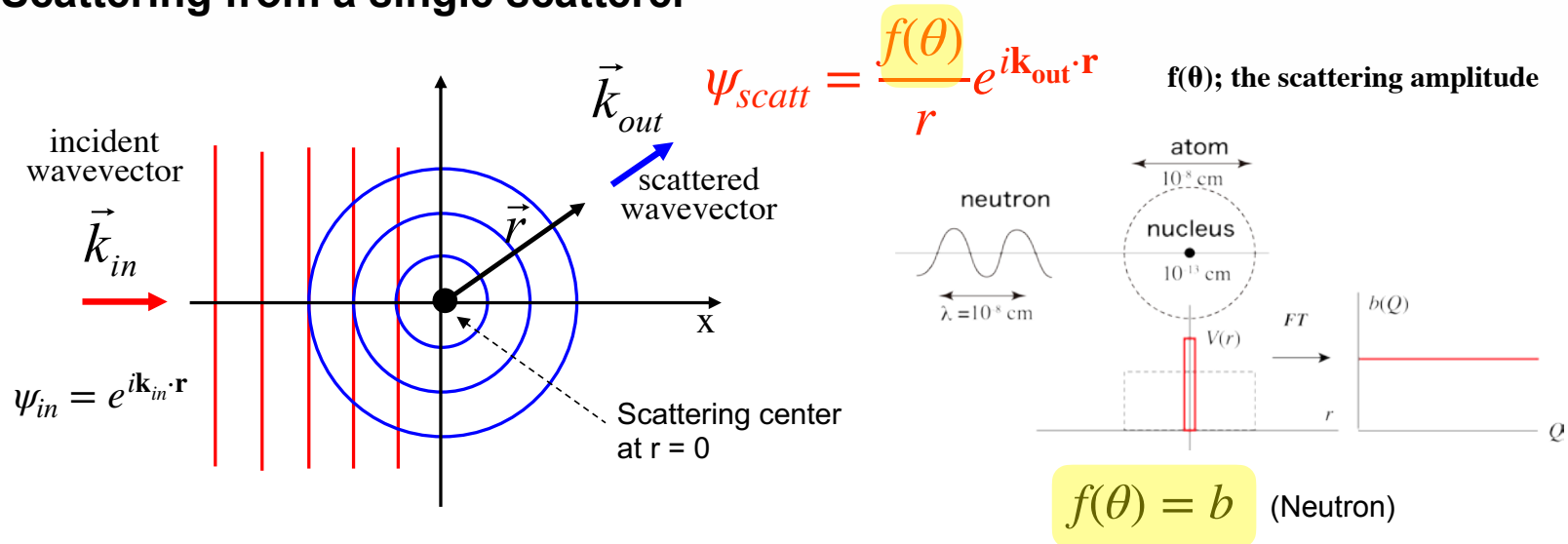
1. Sample environment
2. Topics

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Scattering from a single scatterer; differential cross section

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Scattering from a single scatterer



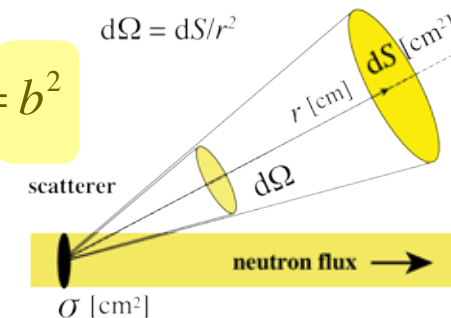
Differential cross section of a single scatterer

Cross section

$$\frac{d\sigma}{d\Omega} = \frac{(\text{no. scatt. neutrons} / sd\Omega)}{v\Phi} = \frac{v|\psi_{scatt}|^2 dS}{vd\Omega} = \frac{vb^2 d\Omega}{vd\Omega} = b^2$$

Solid angle

$\Phi = v|\psi_{in}|^2$; incident flux of neutron
; v the velocity of neutron

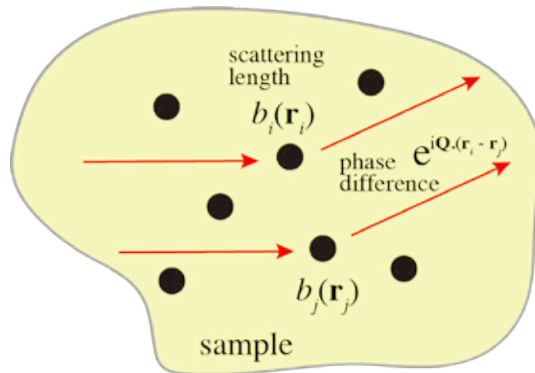


From single scatterer to many scatterers; scattering vector

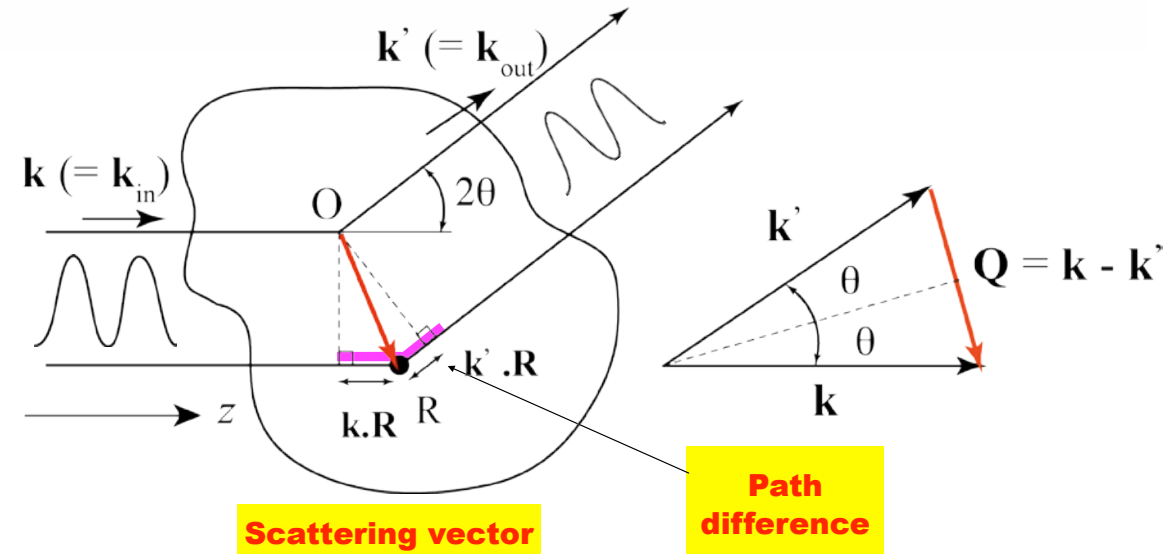
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Single nucleus (molecule)

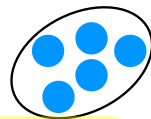
$$\frac{d\sigma}{d\Omega} = |f|^2 = b^2$$



Definition of “scattering vector”



Many nuclei (molecules)



$$\left(\frac{d\sigma}{d\Omega} \right)_N = \frac{1}{N} \left\langle \sum_i^N \sum_j^N b_i(\mathbf{r}_i) b_j(\mathbf{r}_j) e^{i\mathbf{Q} \cdot (\mathbf{r}_i - \mathbf{r}_j)} \right\rangle = \frac{1}{N} \left\langle \left| \sum_j^N b_j(\mathbf{r}_j) e^{i\mathbf{Q} \cdot \mathbf{r}_j} \right|^2 \right\rangle$$

$$\begin{aligned} \mathbf{Q} &= \mathbf{k}_{in} - \mathbf{k}_{out} = \mathbf{k} - \mathbf{k}' \\ &= \mathbf{k} \cdot \mathbf{R} - \mathbf{k}' \cdot \mathbf{R} = (\mathbf{k} - \mathbf{k}') \cdot \mathbf{R} \end{aligned}$$

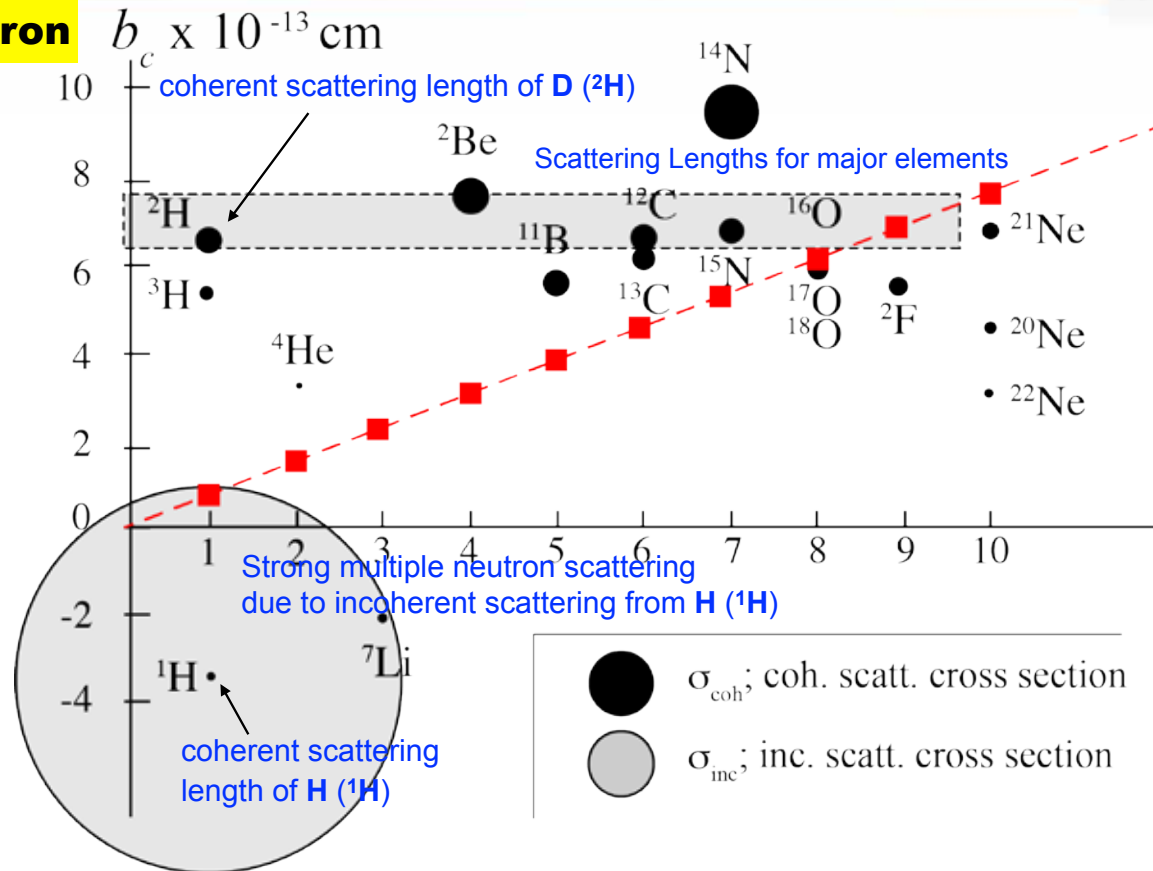
$$Q = |\mathbf{Q}| = 2k \sin \theta = \frac{4\pi}{\lambda} \sin \theta$$

“ruler” 

Scattering length: neutron vs X-ray

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Neutron



X-ray

$b_c, \text{X-ray}$

$$b \propto Z$$

Scattering
(Structure/dynamics)

Z Atomic number

Scattering
(H/D labeling)

Detector

Contrast: Scattering length density (SLD)

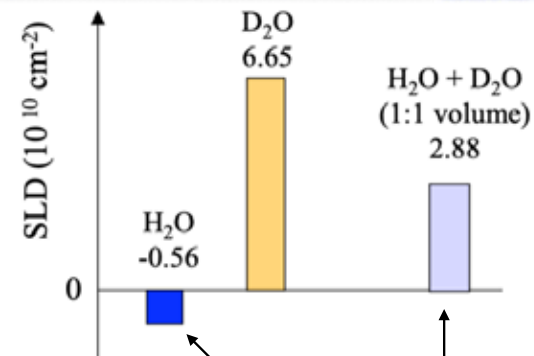
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Scattering length

$$b = b_{\text{molecule}} \sum_j^{(\text{molecule})} n_j b_{(\text{atom}),j} \quad [\text{cm}] \quad \text{Unit: cm}$$

Scattering length density (SLD)

$$\beta \equiv \frac{b_{\text{molecule}}}{v_{\text{molecule}}} \quad [\text{cm}^{-2}] \quad \text{Unit: cm}^{-2}$$



Isotope	conc	Coh b	Inc b	Coh xs	Inc xs	Scatt xs	Abs xs
	%	fm (=10 ⁻¹³ cm)	fm	barn(=10 ⁻²⁴ cm ²)	barn	barn	barn
isotope	Conc.	Coh. Scatt. length	Inc. scatt. length	Coh. Cross section	Inc. cross section	Scattering cross section	Absorption cross section
H	---	-3.739	---	1.7568	80.26	82.02	0.3326
¹ H	99.985	-3.7406	25.274	1.7583	80.27	82.03	0.3326
² H	0.015	6.671	4.04	5.592	2.05	7.64	0.000519
C	---	6.646	---	5.551	0.001	5.551	0.0035
N	---	9.36	---	11.01	0.5	11.51	1.9
O	---	5.803	---	4.232	0.0008	4.232	0.00019

b

σ_{coh}

σ_{inc}

σ_s

σ_a

<http://www.ncnr.nist.gov/resources/n-lengths/>

Molecular scattering length and SLD

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Scattering length

$$b \equiv b_{\text{molecule}} = \sum_i n_i b_{\text{atom},i}$$

Ex.: H₂O; $2 \times \overset{b_H}{(-3.739 \times 10^{-13})} + \overset{b_O}{5.803 \times 10^{-13}} = -1.675 \times 10^{-13} \text{ [cm]}$
 D₂O; $2 \times \overset{b_D}{(+6.671 \times 10^{-13})} + \overset{b_O}{5.803 \times 10^{-13}} = 19.145 \times 10^{-13} \text{ [cm]}$

Scattering length density (SLD)

$$\beta = \frac{\rho N_A}{m} \sum_{j=1}^K (\text{num})_j \langle b \rangle_j$$

Ex.: SLD of H₂O

H₂O; $m = 18.02 \text{ g mol}^{-1}$, $\rho = 1.00 \text{ g cm}^{-3}$

$$\beta = \frac{\rho N_A}{m} \sum_{j=1}^K (\text{num})_j \langle b \rangle_j = \frac{\rho N_A}{m} \sum_{j=1}^K (\text{num})_j \langle b \rangle_{\text{Si}}$$

$$= \frac{(1.00 \times 10^{-24}) \times 6.02 \times 10^{23} \times (-1.675) \times 10^{-5}}{18.0}$$

$$\beta = -5.62 \times 10^{-7} \text{ \AA}^{-2}$$

$10^{-13} \text{ cm} \rightarrow \text{\AA}$

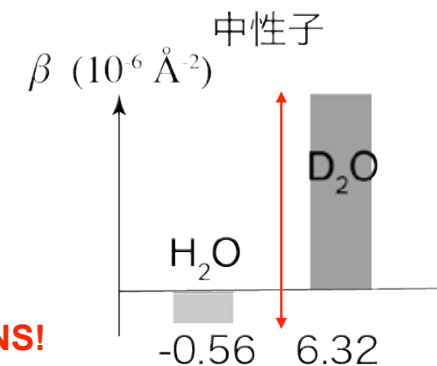
Ex.: SLD of D₂O

D₂O; $m = 20.02 \text{ g mol}^{-1}$, $\rho = 1.10 \text{ g cm}^{-3}$

$$\beta = \frac{\rho N_A}{m} \sum_{j=1}^K (\text{num})_j \langle b \rangle_j = \frac{\rho N_A}{m} \sum_{j=1}^K (\text{num})_j \langle b \rangle_{\text{Si}}$$

$$= \frac{(1.10 \times 10^{-24}) \times 6.02 \times 10^{23} \times (19.1) \times 10^{-5}}{20.0}$$

$$\beta = 6.32 \times 10^{-6} \text{ \AA}^{-2}$$



Very large contrast between D₂O and H₂O in SANS!

Cf. SLDs of X-ray

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Simply substitute scattering length $\langle b \rangle_j$ by atomic number Z_j and Thomson scattering length r_e .

$$\langle b \rangle_j \rightarrow Z_j r_e$$

$$\beta = \frac{\rho N_A}{m} \sum_{j=1}^K (\text{num})_j Z_j r_e$$

$$r_e = 2.82 \times 10^{-5} \text{ \AA}$$

Ex.: X-ray SLD of H₂O

H₂O; $m = 18.02 \text{ g mol}^{-1}$, $\rho = 1.00 \text{ g cm}^{-3}$

$$\sum_{j=1}^K (\text{num})_j Z_j = (1 \times 2 + 16) = 18$$

$$\beta = \frac{\rho N_A}{m} \sum_{j=1}^K (\text{num})_j Z_j r_e$$

$$= \frac{(1.00 \times 10^{-24}) \times 6.02 \times 10^{23} \times 18 \times 2.82 \times 10^{-5}}{18.0}$$

$$\beta = 1.70 \times 10^{-5} \text{ \AA}^{-2}$$

Ex.: X-ray SLD of D₂O

D₂O; $m = 20.02 \text{ g mol}^{-1}$, $\rho = 1.10 \text{ g cm}^{-3}$

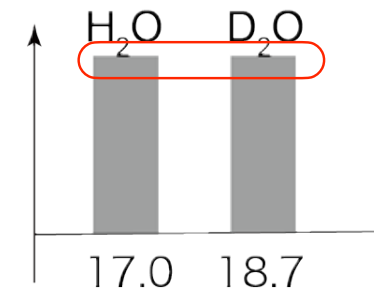
$$\sum_{j=1}^K (\text{num})_j Z_j = (2 \times 2 + 16) = 20$$

$$\beta = \frac{\rho N_A}{m} \sum_{j=1}^K (\text{num})_j Z_j r_e$$

$$= \frac{(1.10 \times 10^{-24}) \times 6.02 \times 10^{23} \times 20 \times 2.82 \times 10^{-5}}{20.0}$$

$$\beta = 1.87 \times 10^{-5} \text{ \AA}^{-2}$$

$\beta \text{ (} 10^{-6} \text{ \AA}^{-2} \text{)}$ X線



Negligible contrast between D₂O and H₂O in SAXS!

From single scatterer, to many scatterers, and macroscopic differential cross section

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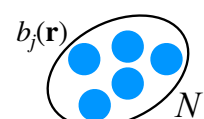
$$\frac{d\sigma}{d\Omega} = |f|^2 = b^2 \quad \text{Single nucleus (molecule)}$$

$[cm^2]$

$$\left(\frac{d\sigma}{d\Omega}\right)_N = \frac{1}{N} \left\langle \sum_i^N \sum_j^N b_i(\mathbf{r}_i) b_j(\mathbf{r}_j) e^{i\mathbf{Q} \cdot (\mathbf{r}_i - \mathbf{r}_j)} \right\rangle = \frac{1}{N} \left\langle \left| \sum_j^N b_j(\mathbf{r}_j) e^{i\mathbf{Q} \cdot \mathbf{r}_j} \right|^2 \right\rangle \quad \text{Many nuclei (molecules)}$$

$$\sum_j^N b_j \rightarrow \int_{V_P} \beta(\mathbf{r}) d^3\mathbf{r} \quad \text{From discrete to continuous}$$

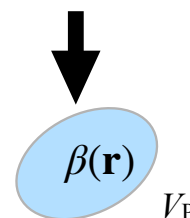
$b [cm] \rightarrow \beta [cm^{-2}]$



$$\left(\frac{d\sigma}{d\Omega}\right)_N = \frac{1}{N} \langle b \rangle^2 \sum_{i,j} e^{i\mathbf{Q} \cdot (\mathbf{r}_i - \mathbf{r}_j)} + N(\langle b^2 \rangle - \langle b \rangle^2)$$

Coherent **incoherent**

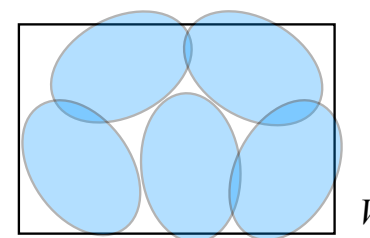
$$\left(\frac{d\sigma}{d\Omega}\right)_{V_P} = \left| \int_{V_P} \beta(\mathbf{r}) e^{i\mathbf{Q} \cdot \mathbf{r}} d^3\mathbf{r} \right|^2 \quad \text{From SL to SLD}$$



$$\left(\frac{d\Sigma}{d\Omega}\right) = \frac{N}{V} \left(\frac{d\sigma}{d\Omega}\right) = n_P \left(\frac{d\sigma}{d\Omega}\right)$$

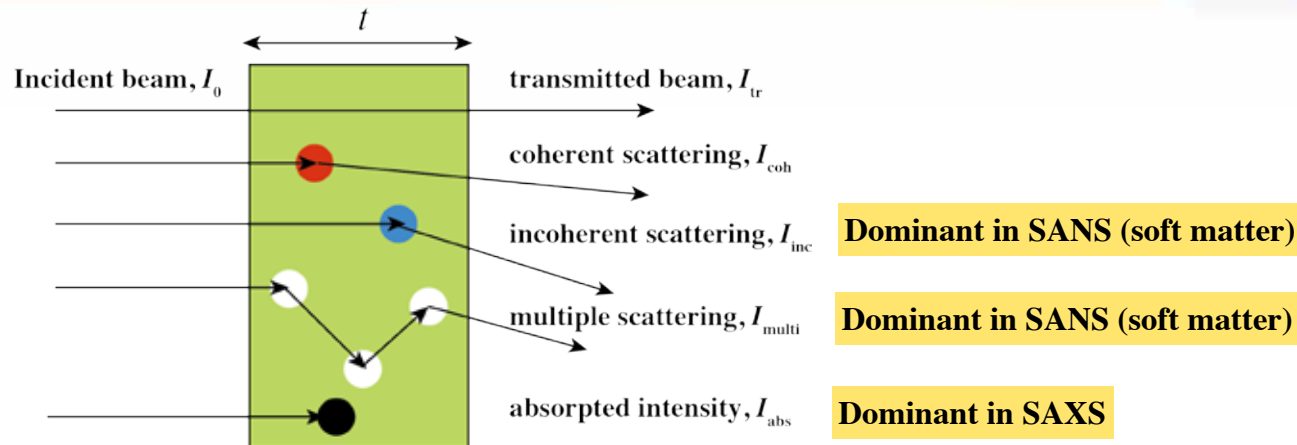
$[cm^{-1}]$ $[cm^2]$

Macroscopic diff. Cross. Section
(Absolute scattering intensity)



Transmission and absorption

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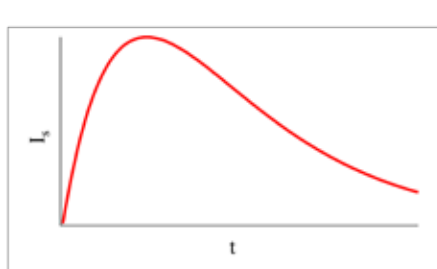
$$f(t) = \Sigma t \exp(-\Sigma t)$$

$$\frac{df(t)}{dt} = [\Sigma + \Sigma t(-\Sigma)] \exp(-\Sigma t) = 0$$

$$\therefore t_{\max} = \frac{1}{\Sigma} = \frac{1}{\rho_N \sigma} [\text{cm}]$$

$$T = \frac{I_{tr}}{I_0} = \exp(-\Sigma_T t) \quad \Sigma_T = \Sigma_{coh} + \Sigma_{inc} + \Sigma_{abs} = \mu$$

Σ_T : total cross section
 μ : linear absorption coefficient



$$I_s \propto \mu t \exp(-\mu t)$$

$$\frac{dI_s}{dt} = \mu(1 - \mu t)e^{-\mu t} = 0$$

$$t_{\max} = 1/\mu = 1/\Sigma_T$$

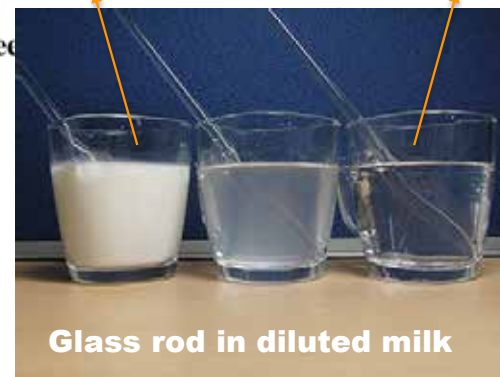
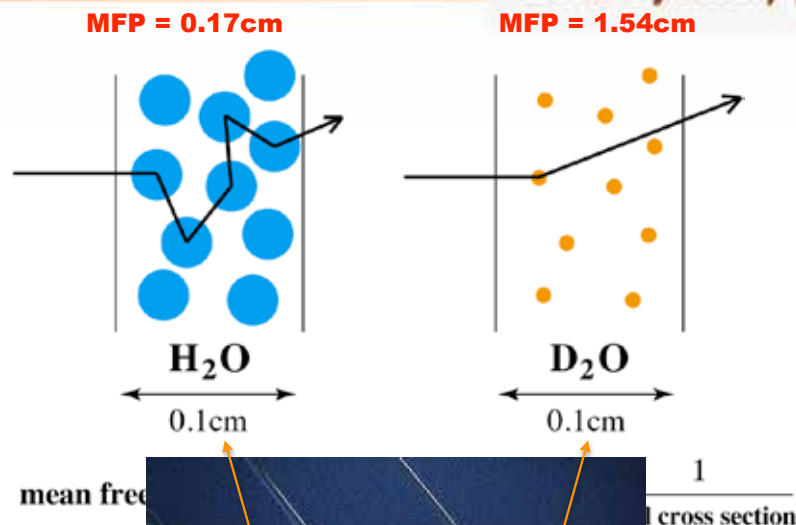
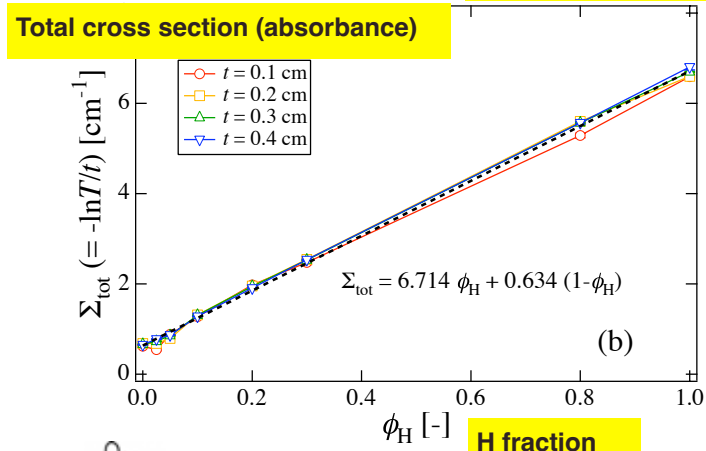
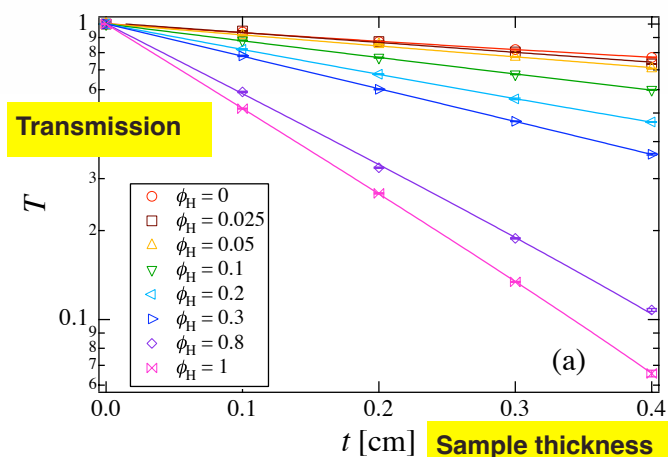
In soft matter
~ 2mm for SAXS,
~ 1mm for SANS

Incoherent scattering and multiple scattering

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J. Appl. Cryst., 2009, 42, 621.

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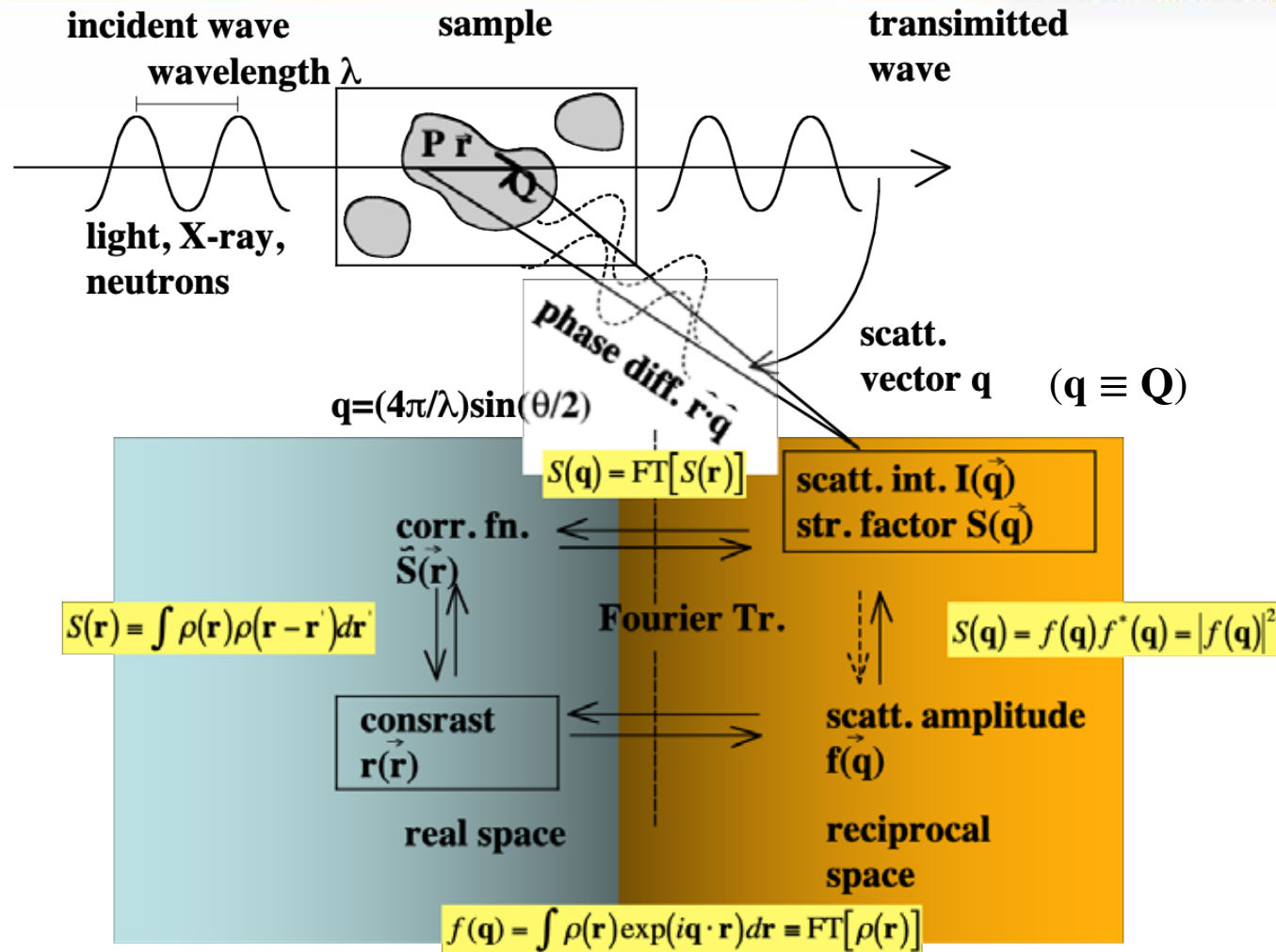
A linear relationship holds all fractions irrespective of sample thickness.



Major cause of attenuation: incoherent scattering (neutron), absorption (X-ray)

Real space vs reciprocal space

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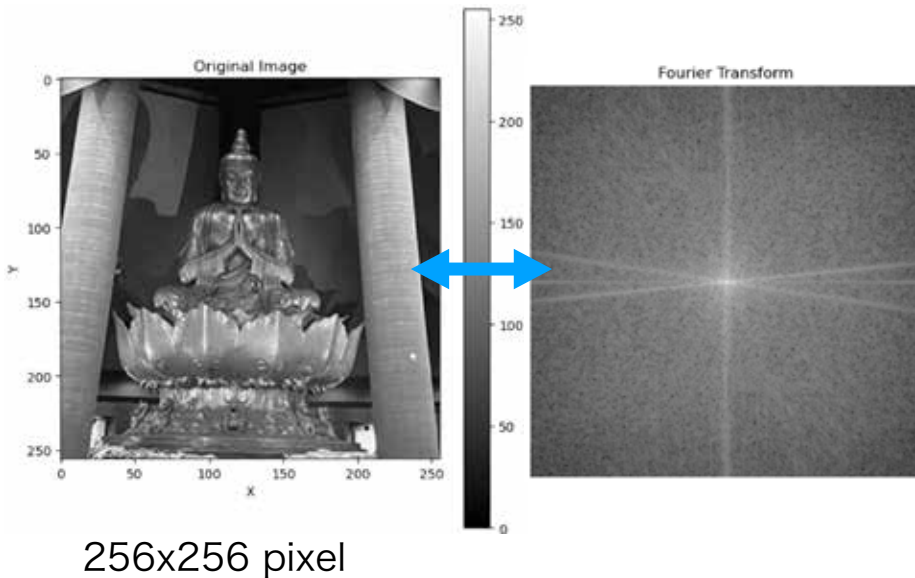


Real vs reciprocal space, filtering

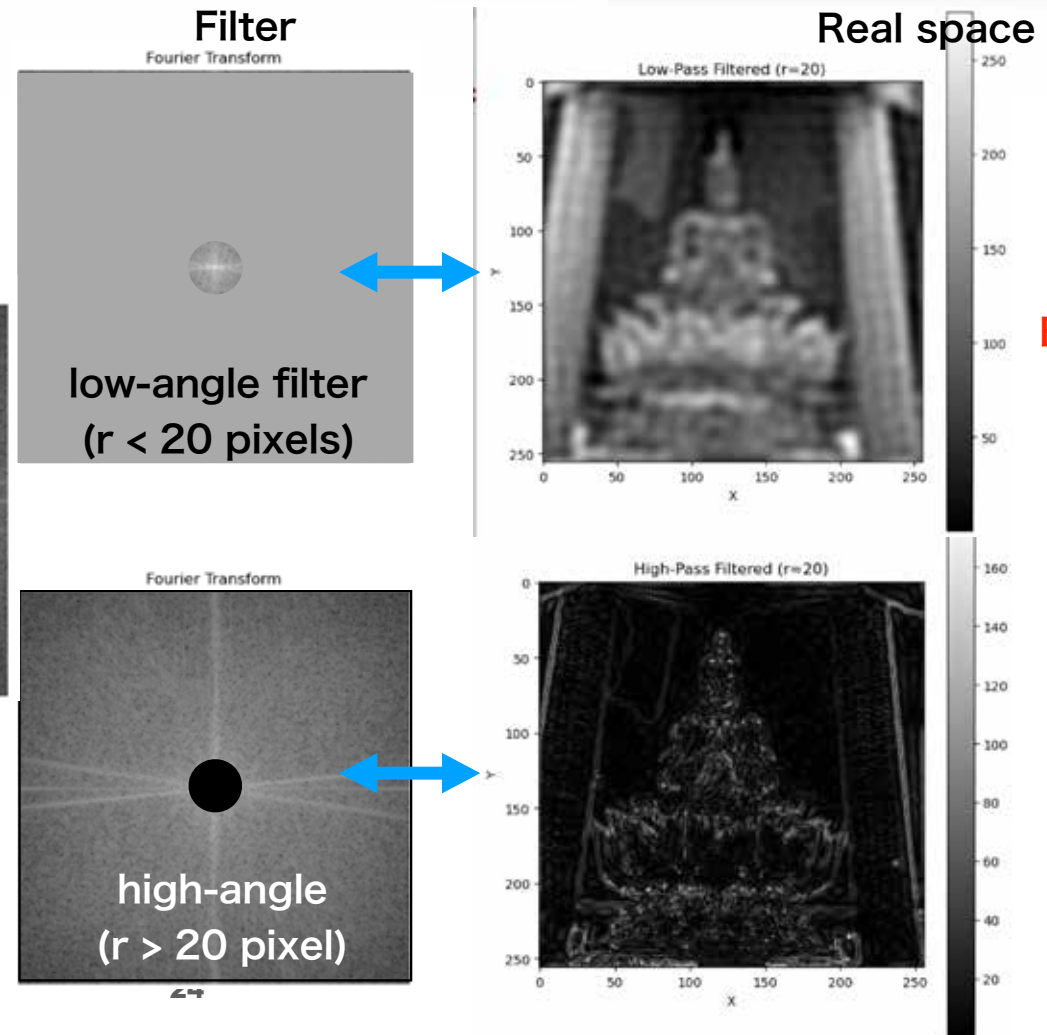
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Fourier transform (FFT) / inverse Fourier transform (IFFT) and filtering

Real space FFT/IFFT Reciprocal space



Real space: Easy to understand intuitively!!
Reciprocal space: No idea what it means? ?



Details are
Blurred.

Details are
Clear.

Summary (Part 2) : important variables

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Scattering length	$b[\text{cm}]$	
Differential cross section	$\frac{d\sigma}{d\Omega}[\text{cm}^2] = b^2$	(single nuclear scattering)
Cross section	$\sigma = \int \left(\frac{d\sigma}{d\Omega} \right) d\Omega = 4\pi b^2 [\text{cm}^2]$	Unit: cm^2
Scattering length density (SLD)	$\beta = \frac{b_{\text{molecule}}}{V_{\text{molecule}}} [\text{cm}^{-2}]$	Unit: cm^{-2}
Absolute intensity	$\frac{d\Sigma}{d\Omega} [\text{cm}^{-1}] = \frac{N}{V} \frac{d\sigma}{d\Omega} = \rho_N \frac{d\sigma}{d\Omega}$	Unit: cm^{-1}
Transmission	$T \equiv \frac{\Phi}{\Phi_0} = \frac{I_{\text{tr}}}{I_0} = e^{-\mu t}$	$(\mu = \sigma \rho_N = \Sigma)$
Scattering amplitude	$I_s \propto \frac{d\Sigma}{d\Omega} \propto I_0 e^{-\Sigma t} \Sigma t$	Product of transmission, cross section, and thickness

Contents

CUHK Lecture, M. Shibayama
2025.8.10 - 16

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1. SANS in Material sciences
2. SANS instruments
3. Angle dispersion vs TOF measurements

Part 2. Basics of Neutron scattering

Part 3. SANS theory

1. Guinier law
2. Form factors (sphere, cylinder, etc.)
3. Porod law
4. Polymer
5. Interacting systems
6. One-phase systems (Ornstein-Zernike)
7. Multi-phase systems (Debye-Bueche)
6. Fractals
8. Asymptotic behaviors

Part 4. Analysis

1. Q-space analysis
2. Corrections
3. real space analysis

Part 5. Applications and Topics

1. Sample environment
2. Topics

Part 6. Summary and reference

Scattering amplitude, scattering intensity

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Scattering amplitude FT of SLD!!

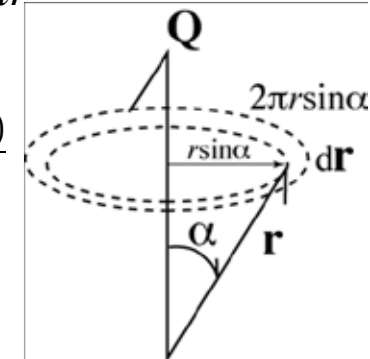
$$f(Q) \equiv \int_{V_p} \underbrace{\Delta\beta(r)}_{\text{SLD}} e^{i\mathbf{Q}\cdot\mathbf{r}} d^3r \quad f(Q) = \int_{V_p} \Delta\beta(r) e^{i\mathbf{Q}\cdot\mathbf{r}} d^3r = \int_0^R 4\pi r^2 \Delta\beta(r) \frac{\sin(Qr)}{Qr} dr$$

$$d\mathbf{r} = d^3r = 2\pi r \sin\alpha dr$$

Differential cross section

$$\frac{d\sigma}{d\Omega} = |f(Q)|^2$$

$$\langle e^{i\mathbf{Q}\cdot\mathbf{r}} \rangle \equiv \frac{\int_0^\pi e^{iQr\cos\alpha} (2\pi r \sin\alpha) d\alpha}{\int_0^\pi 2\pi r \sin\alpha d\alpha} = \frac{2 \sin(Qr)/Qr}{[-\cos\alpha]_0^\pi} = \frac{\sin(Qr)}{Qr}$$



Scattering intensity

$$\frac{d\Sigma}{d\Omega} = n_p |f(Q)|^2$$

Macroscopic diff. Cross section
(Absolute scattering intensity)

$$\langle e^{i\mathbf{Q}\cdot\mathbf{r}} \rangle = \frac{\sin(Qr)}{Qr}$$

$$\frac{\sin x}{x} = \frac{1}{x} \left[x - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} + \dots \right] = 1 - \frac{x^2}{6} + \frac{x^4}{120} - \frac{x^6}{7!} + \dots$$

Guinier law: SAS law of dilute systems

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Scattering amplitude

Unit: cm

$$f(Q) = \int_{V_p} \Delta\beta(r) e^{i\mathbf{Q}\cdot\mathbf{r}} d^3r = \int_0^R 4\pi r^2 \Delta\beta(r) \frac{\sin(Qr)}{Qr} dr$$

$$V_p = \frac{4\pi}{3} R^3$$

$$= (\Delta\beta) \int_0^R 4\pi r^2 \left[1 - \frac{Q^2}{6} r^2 + \dots \right] dr \quad \because \langle e^{i\mathbf{Q}\cdot\mathbf{r}} \rangle_{\text{orient}} = \frac{\sin(Qr)}{Qr} = 1 - \frac{1}{3!}(Qr)^2 + \frac{1}{5!}(Qr)^4 - \dots$$

$$= (\Delta\beta) \left[V_p - \frac{Q^2}{6} 4\pi \frac{1}{5} R^5 + \dots \right] = (\Delta\beta) V_p \left[1 - \frac{Q^2}{6} R_g^2 + \dots \right]$$

$$R_g^2 \equiv \frac{\int_{V_p} r^2 d^3r}{\int_{V_p} d^3r} = \frac{3}{5} R^2$$



A. Guinier

Scattering intensity (differential cross section per unit volume)

Unit: cm⁻¹

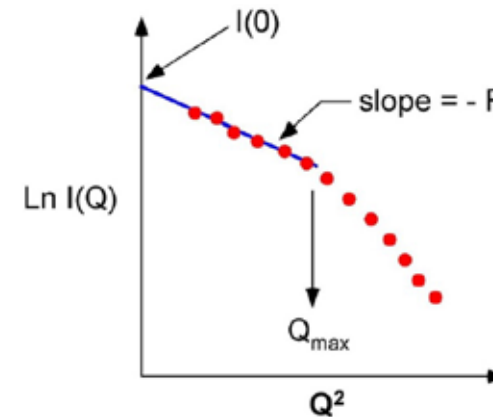
n_p : number density of the scatterers

$$\frac{d\Sigma}{d\Omega} \equiv n_p |f(Q)|^2 = n_p V_p^2 (\Delta\beta)^2 \left[1 - \frac{R_g^2 Q^2}{6} + \dots \right]^2$$

$$= n_p V_p^2 (\Delta\beta)^2 \exp\left[-\frac{R_g^2 Q^2}{3}\right]$$

Guinier law

$$\frac{d\Sigma}{d\Omega} \propto \exp\left[-\frac{R_g^2 Q^2}{3}\right]$$



$$Q_{\max} R_g \leq 1$$

Scattering from a single sphere

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Scattering intensity from a single sphere

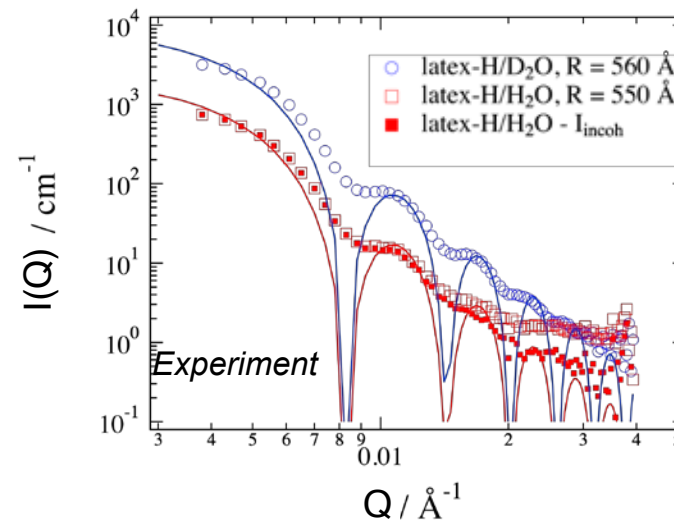
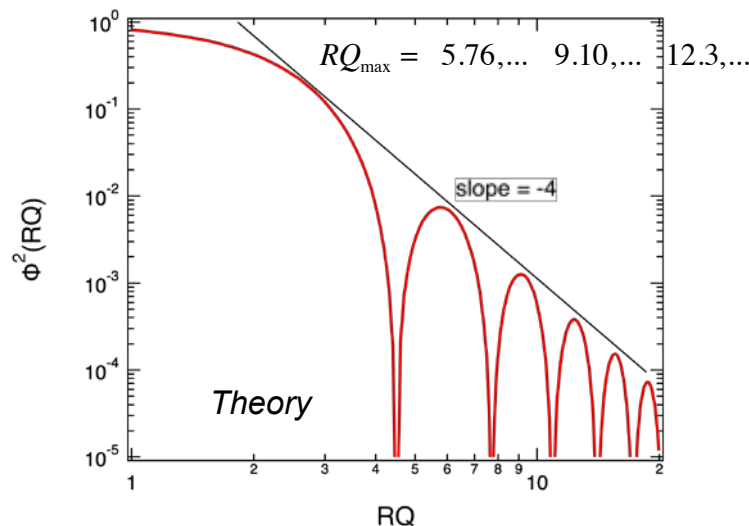
with radius R , volume V_p , and the scattering length density (SLD) β

$$\left(\frac{d\sigma}{d\Omega}\right) = |f(Q)|^2 = \left(\frac{4\pi R^3}{3}\right)^2 \beta^2 \Phi^2(U) = \beta^2 V_p^2 \Phi^2(U)$$

$$U \equiv RQ, \Phi(U) \equiv \frac{3}{U^3}[\sin U - U \cos U]$$

The intensity is proportional to the square of V and the square of SLD.

$$\left(\frac{d\sigma}{d\Omega}\right) \propto \Phi^2(U) \propto Q^{-4} \quad (Q \rightarrow \infty)$$



The intensity from a sphere is proportional to V_p^2 , β^2 , and Q^{-4} .

Guinier law: SAS of dilute systems

$$\left(\frac{d\Sigma}{d\Omega}\right) \approx \phi V_P (\beta_P - \beta_0)^2 \left[1 - \frac{R_g^2}{3} Q^2 + \dots\right] \approx \phi V_P (\beta_P - \beta_0)^2 e^{-\frac{R_g^2}{3} Q^2}$$

$$\because N/V = n_p \phi$$

$$\left(\frac{d\Sigma}{d\Omega}\right) \approx \phi V_P (\beta_P - \beta_0)^2 e^{-\frac{R_g^2}{3} Q^2}$$

This is so-called Guinier law, and it shows the behavior of SAS at low Q .

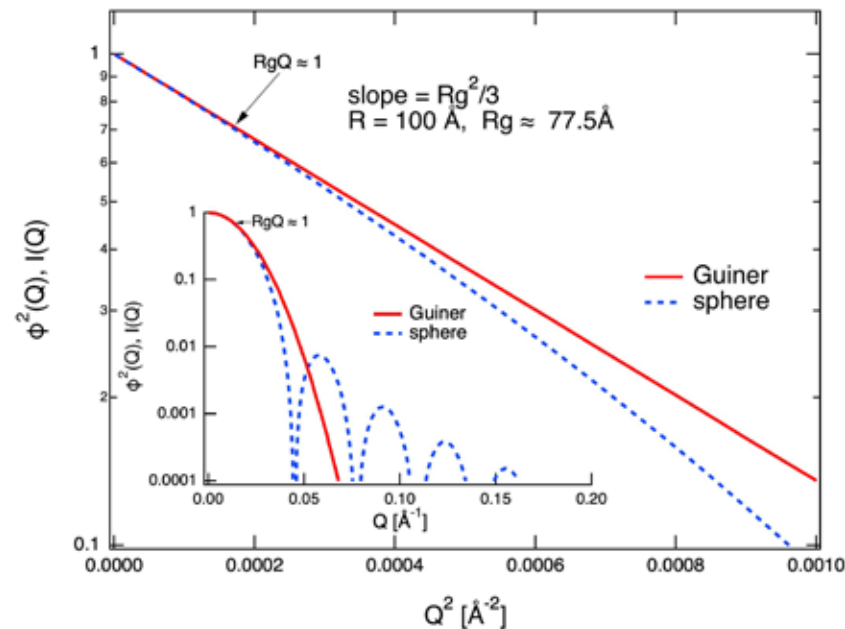
Guinier plot

$$\ln[I(Q)] \approx \ln[I(Q=0)] - \frac{R_g^2}{3} Q^2$$

$$I(Q=0) \equiv \left(\frac{d\Sigma}{d\Omega}\right)_{Q=0}$$

**Conventional method to estimate
The particle size in a dilute system.**

Guinier plot



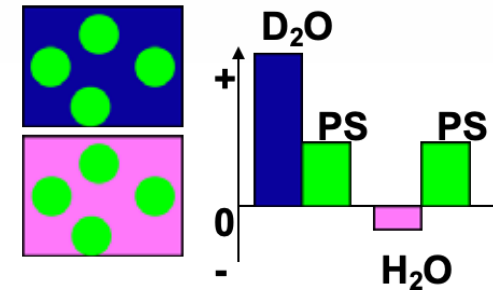
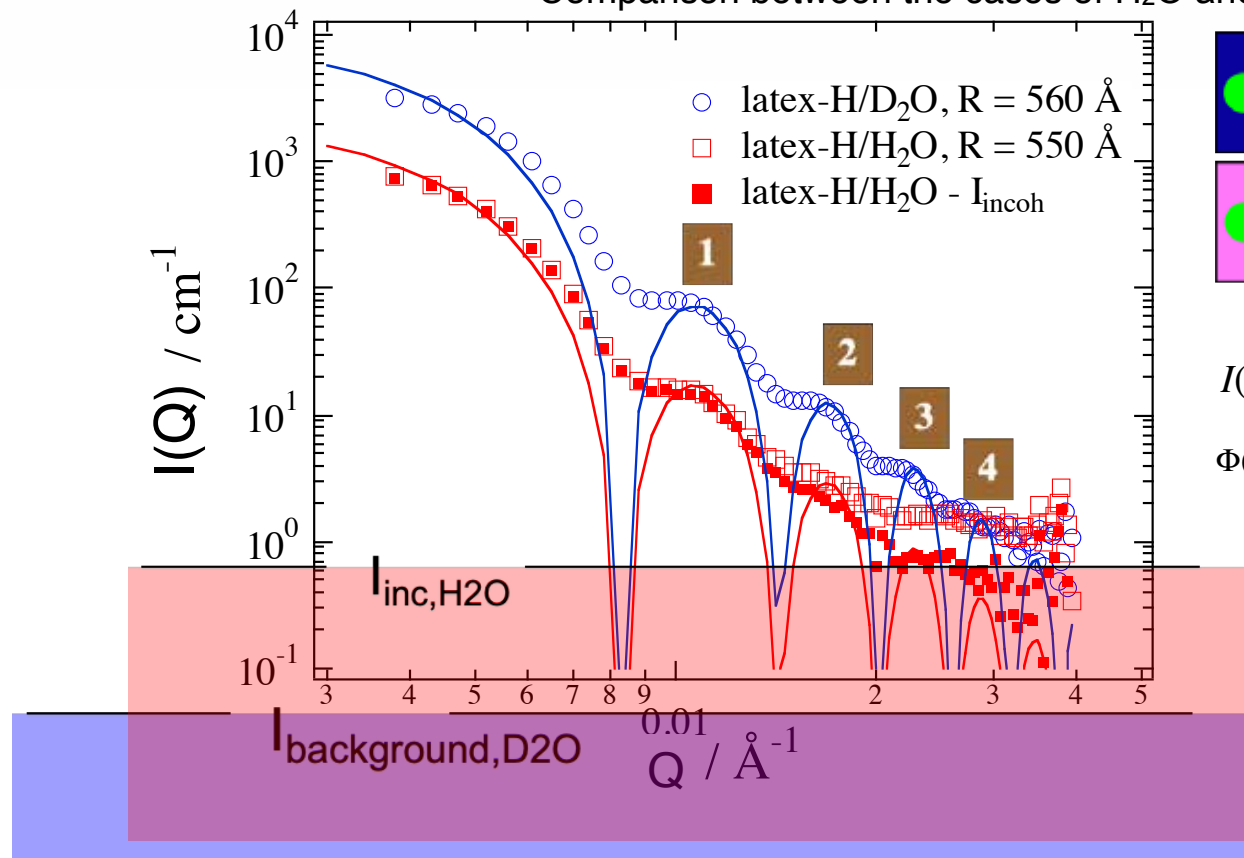
For $R_g = 100 \text{ Å}$, deviation starts to appear at $Q_{\text{dev}} \approx 0.02 \text{ Å}^{-1}$.

As $R_g Q_{\text{dev}}$, deviation becomes clear at $R_g Q_{\text{dev}} \approx 2$.
So, Guinier approximation should apply for $R_g Q_{\text{dev}} < 1$!

Effect of Incoherent scattering: SANS from polystyrene latex

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Comparison between the cases of H₂O and D₂O.



$$I(q) = nV^2(\Delta\beta)^2\Phi^2(Rq)$$

$$\Phi(Rq) = \frac{3[\sin(Rq) - Rq \cos(Rq)]}{(Rq)^3}$$

$$\equiv 3\sqrt{\frac{\pi}{2}} \frac{J_{3/2}(Rq)}{(Rq)^{3/2}}$$



In the case of H₂O, the structure information is buried in incoherent scattering.

Scattering from a spherical core-shell

Shibayama, CROSS

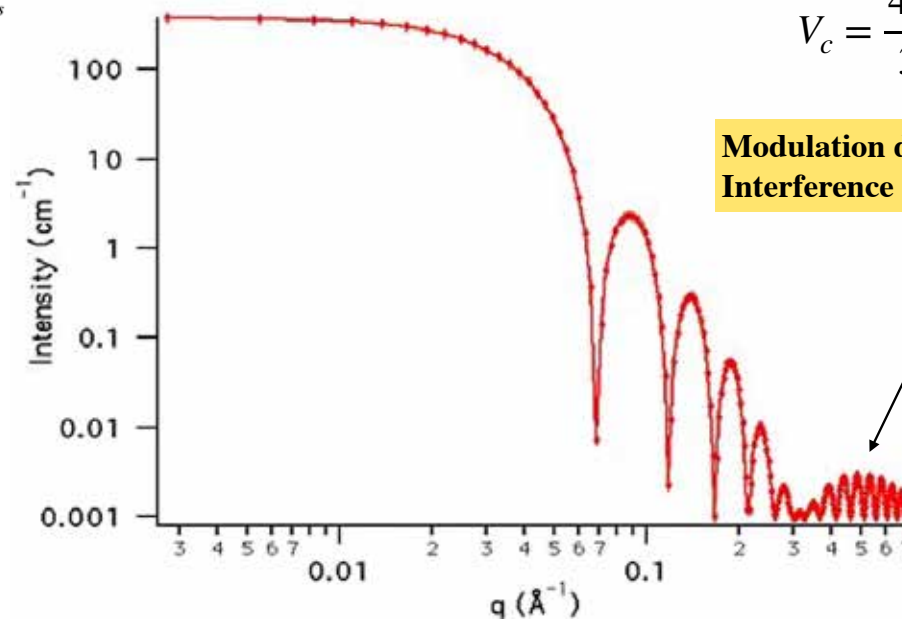
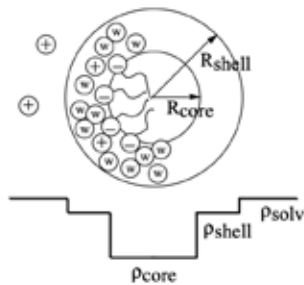
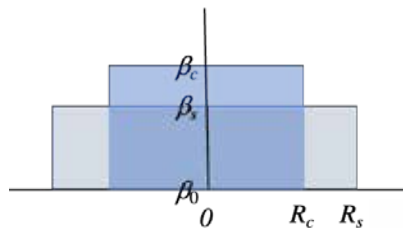
$$\frac{d\Sigma}{d\Omega} = \frac{N}{V} P(Q) = \phi_p V_p |f(Q)|^2$$

$$f(Q) = 3V_c(\beta_c - \beta_s)\Phi(QR_c) + V_s(\beta_s - \beta_0)\Phi(QR_s)$$

core

shell

$$V_c = \frac{4\pi}{3}R_c^3, V_s = \frac{4\pi}{3}R_s^3$$



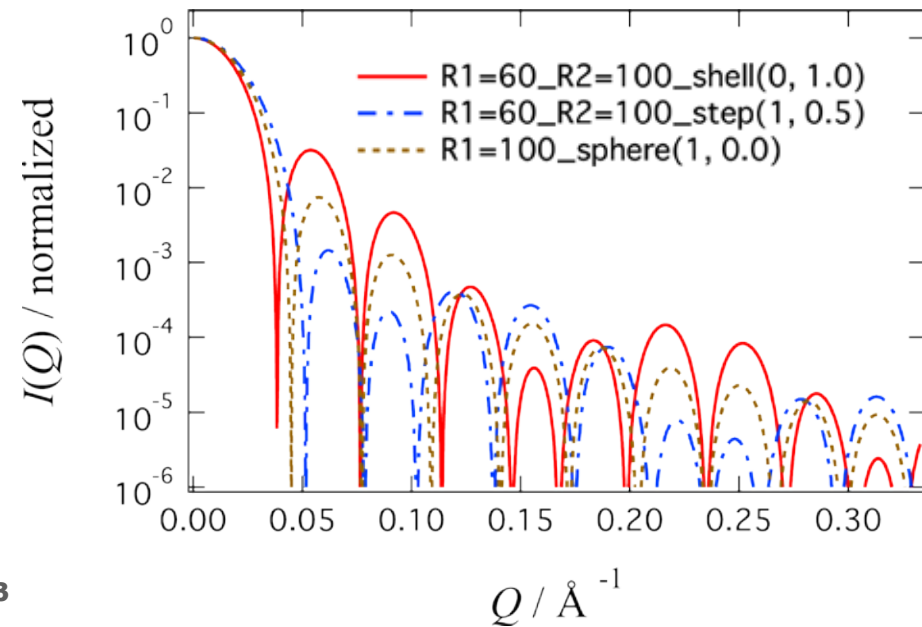
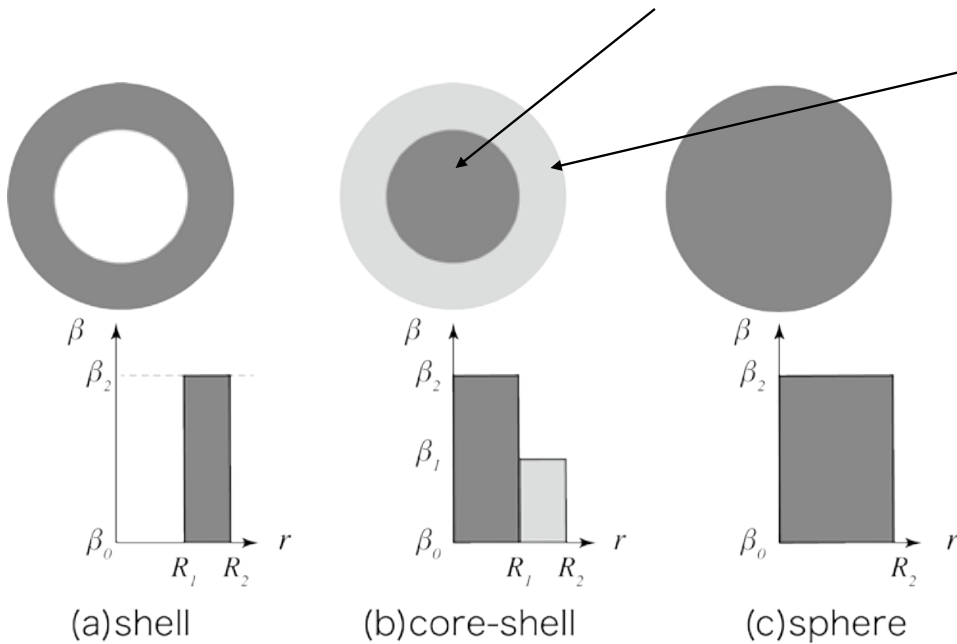
Modulation due to
Interference between core and shell

Shell, core-shell, vs sphere

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$$f(Q) = \int_{V_P} \beta(\mathbf{r}) e^{i\mathbf{Q} \cdot \mathbf{r}} d^3\mathbf{r} = \beta_1 \int_0^{R_1} A dr + \beta_2 \int_{R_1}^{R_2} A dr \quad A \equiv 4\pi r^2 \frac{\sin(Qr)}{Qr}$$

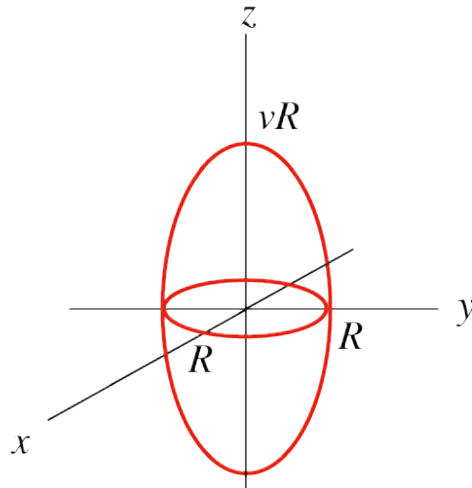
$$\frac{d\sigma}{d\Omega} = |f(Q)|^2 = \left[(\beta_1 - \beta_0) V_{P1} \Phi(U_1) + (\beta_2 - \beta_0) \{ V_{P2} \Phi(U_2) - V_{P1} \Phi(U_1) \} \right]^2$$



Scattering from a rod/disk

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Ellipsoid of revolution



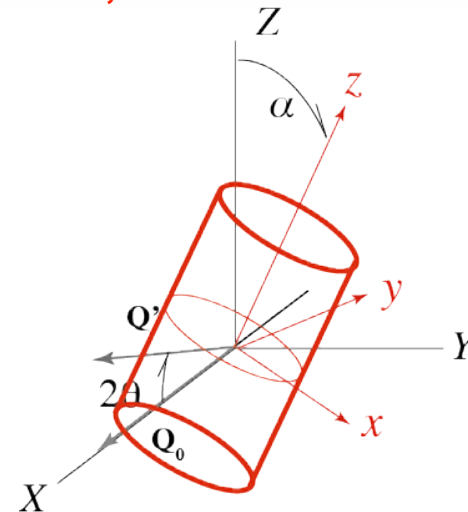
$$\left(\frac{d\sigma}{d\Omega} \right) = V_{\text{ellip}}^2 \beta_{\text{ellip}}^2 \Phi(U^*)^2$$

$$U^* = U_0 [1 + (v^2 - 1) \cos^2 \theta \cos \mu]$$

$$U_0 \equiv RQ$$

v : axial ratio

Cylinder, disk



$$f(Q, \alpha)_{\text{rod}} = \beta_{\text{rod}} V_{\text{rod}} \frac{2J_1(RQ \sin \alpha)}{RQ \sin \alpha} \frac{\sin(LQ \cos \alpha)}{LQ \cos \alpha}$$

$$\left(\frac{d\sigma}{d\Omega} \right) = \left| \int_0^{\pi/2} f(Q, \alpha)_{\text{rod}} \sin \alpha d\alpha / \int_0^{\pi/2} \sin \alpha d\alpha \right|^2$$

(X-axis incidence)

Scattering from an oriented particle

Shibayama, CROSS

$$I(Q) \propto |F(Q)|^2 = \left| \frac{1}{V_p} \int_{V_p} e^{i\mathbf{Q} \cdot \mathbf{r}} d\mathbf{r} \right|^2$$

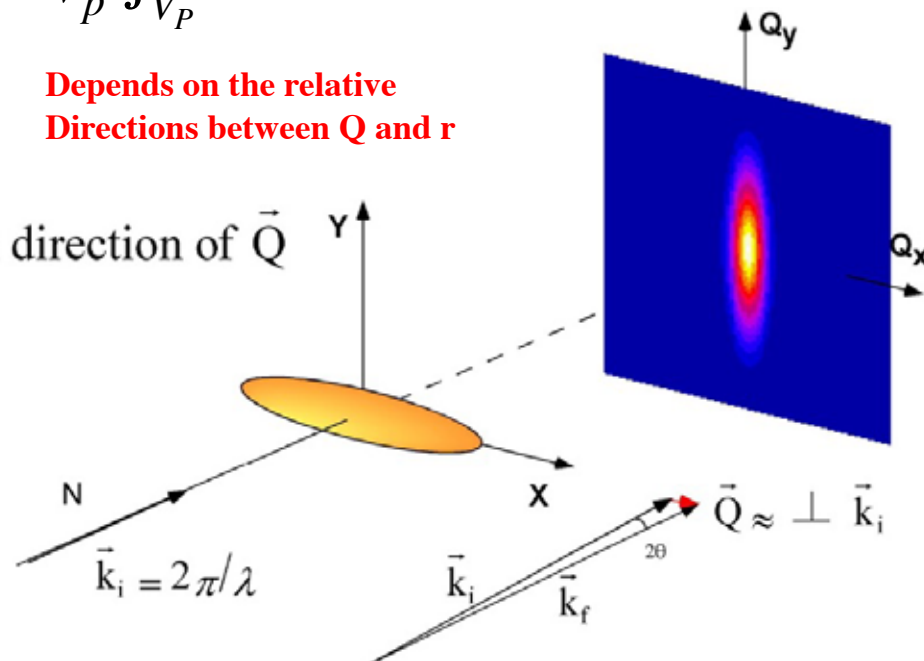
$$\mathbf{Q} \cdot \mathbf{r} = Qr \cos \alpha$$

Depends on the relative
Directions between $\mathbf{Q}$ and $\mathbf{r}$

$I(\vec{Q})$ probes structure in direction of $\vec{Q}$

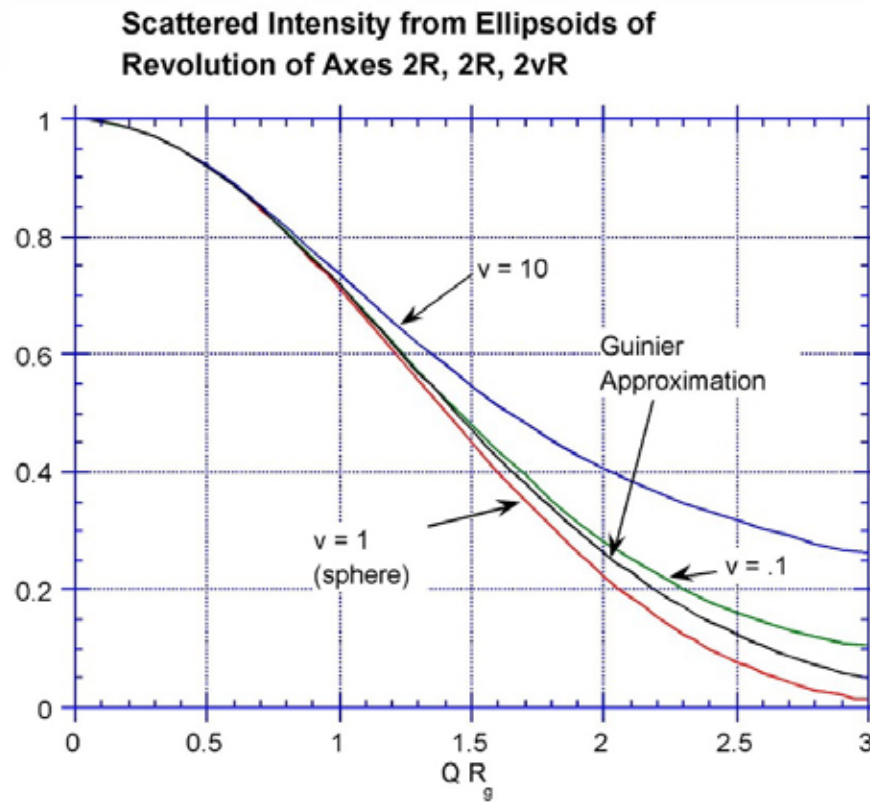
Reciprocal phenomena

$$Q \propto \frac{1}{\text{length}}$$

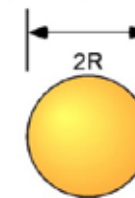


Scattering from a randomly oriented ellipsoid of revolution

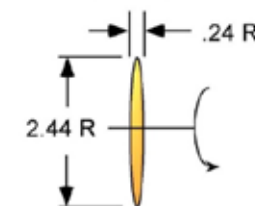
Shibayama, CROSS



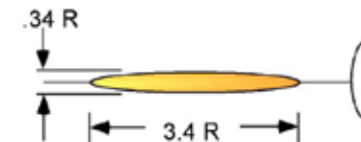
Sphere ($v = 1$)



Oblate Ellipsoid ($v = 1/10$)

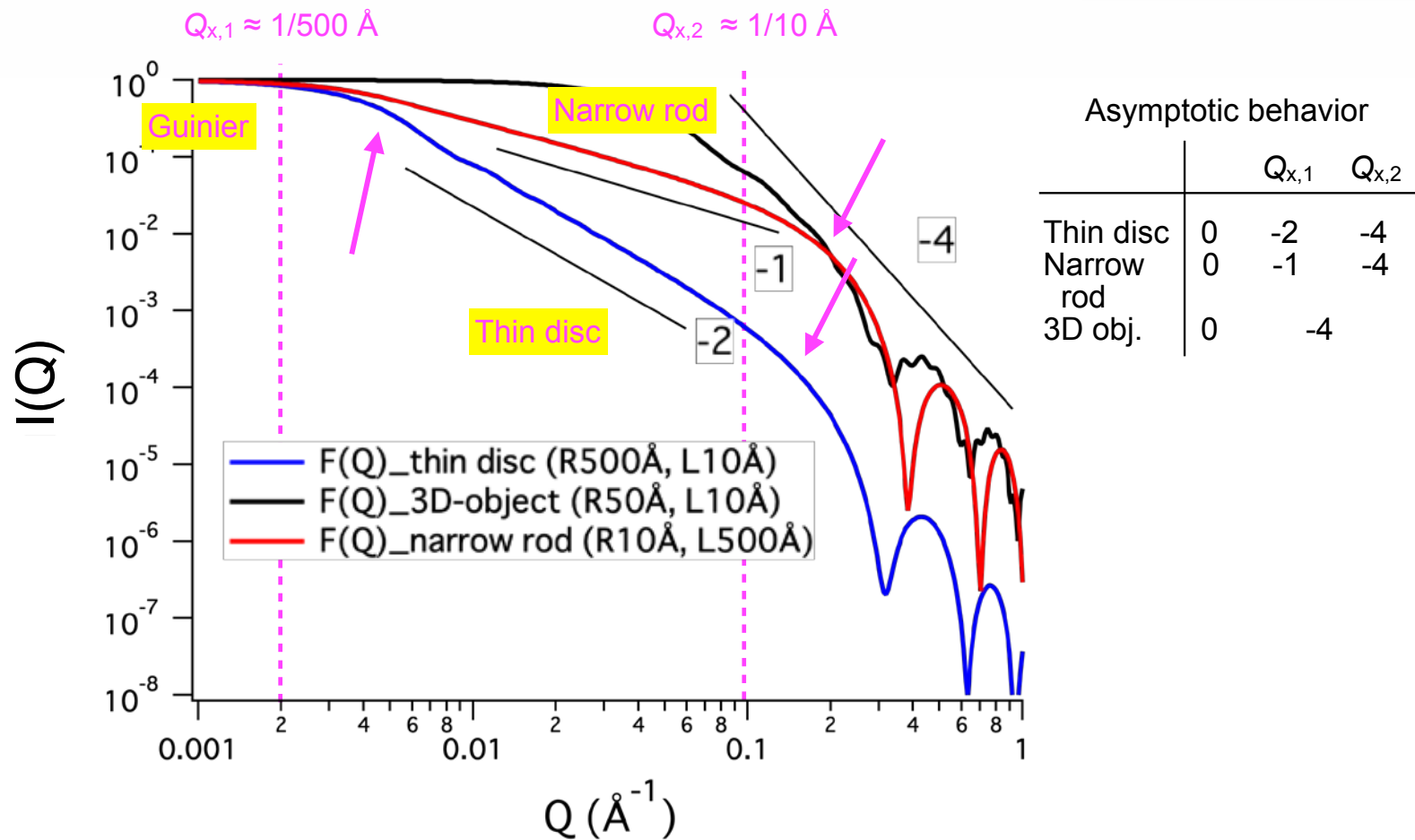


Prolate Ellipsoid ($v = 10$)



Scattering intensity from randomly oriented particles

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Porod law

Shibayama, CROSS

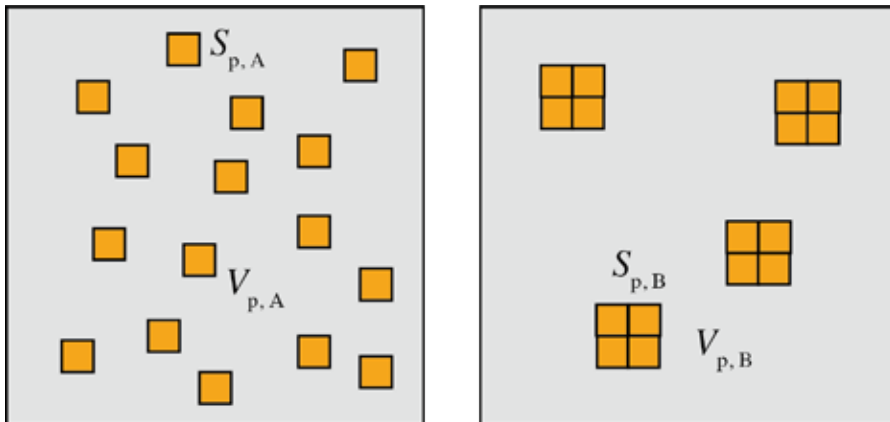
$$I(Q \rightarrow \infty) \propto (\Delta\beta)^2 2\pi S_{sp} Q^{-4}$$

$$I(Q) \propto Q^{-4}$$

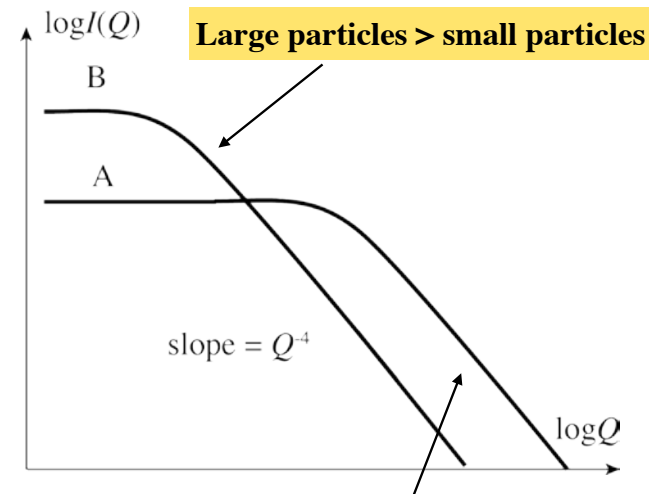
$$S_{sp} \equiv \frac{S_p}{V_p}$$

Specific surface area of sample

S/V = specific surface area of sample



$$S_{p,A} / V_{p,A} > S_{p,B} / V_{p,B}$$



small particles > Large particles

Useful for studying porous materials

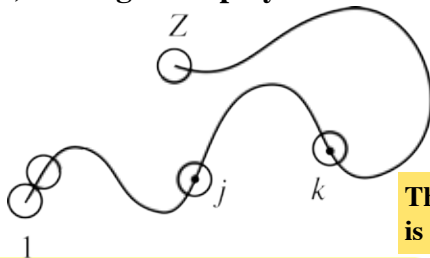
Polymer: scattering function for a Gaussian chain

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Debye function for a polymer chain

$$g_D(Q) = \int d\mathbf{r} e^{i\mathbf{Q} \cdot \mathbf{r}} = \frac{1}{Z} \sum_{j=1}^Z \sum_{k=1}^Z \langle e^{i\mathbf{Q} \cdot (\mathbf{r}_j - \mathbf{r}_k)} \rangle$$

Z ; the degree of polymerization



The scattering element is each monomer!

$$g_D(Q) = \frac{2Z}{u^2} [e^{-u} - 1 + u]$$

$$u \equiv R_g^2 Q^2 \quad R_g^2 = \frac{Za^2}{6}$$



a ; monomer length

$$g_D(Q) \approx Z[1 - \frac{R_g^2 Q^2}{3}], (R_g Q \ll 1)$$

$$g_D(Q \rightarrow \infty) \propto \frac{2Z}{R_g^2 Q^2}, (R_g Q \gg 1)$$

Scattering intensity of a single polymer chain

$$\left(\frac{d\sigma}{d\Omega} \right) = b_m^2 g_D(Q)$$

b_m ; the scattering length of the monomer

Scattering intensity of a polymer solution

$$\begin{aligned} \left(\frac{d\Sigma}{d\Omega} \right) &= \phi_p (\beta_p - \beta_s)^2 v_m g_D(Q) \\ &= \phi_p (\beta_p - \beta_s)^2 v_m Z \frac{2}{u^2} [e^{-u} - 1 + u] \end{aligned}$$

Intensity is proportional to the degree of polymerization, Z

v_m ; the monomer volume

ϕ_p ; the polymer volume fraction

$$\left(\frac{d\Sigma}{d\Omega} \right)_{Q=0} = \phi_p (\beta_p - \beta_s)^2 v_m Z$$

SAS is used to evaluate the molecular weight.

Polymer chains in solution, polymer blends

Shibayama, CROSS

Polymer solution (Zimm equation)

$$\frac{HC}{d\Sigma/d\Omega} = \frac{1}{M_w} \left[1 + \frac{R_g^2}{3} Q^2 + \dots \right] + 2A_2C + \dots$$

$$H = N_{av} \frac{(\beta_p - \beta_s)^2}{\rho^2} \rightarrow M_w, R_g, A_2$$

M_w ; the molecular weight, N_{av} ; the Avogadro number,
 A_2 ; the second virial coefficient

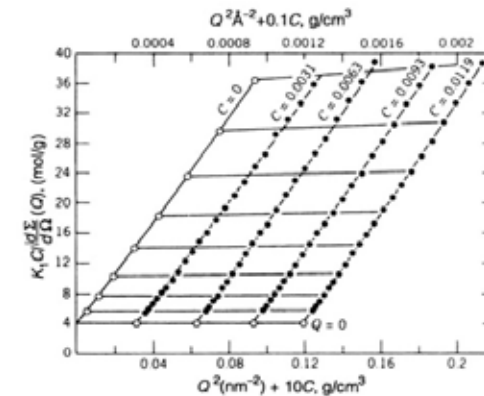


Fig. 8.2 Zimm plot of data in Fig. 8.1. The open circles are the result of extrapolation to zero C and zero Q ($= q$) (Kirste *et al.* 1975). Reprinted with permission from Wignall (1987).

Polymer blend (Random phase approximation, RPA)

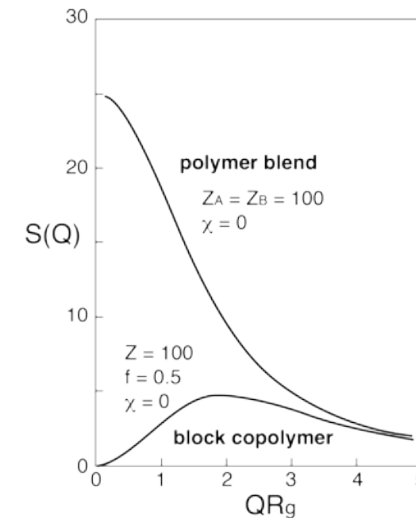
$$\frac{1}{v_0 S(Q)} = \frac{1}{v_A \phi_A g_D(Q; Z_{P,A})} + \frac{1}{v_B \phi_B g_D(Q; Z_{P,B})} - 2 \frac{\chi}{v_0}$$

$$g_{D,i}(Q; Z_{P,i}) \equiv \frac{2Z_{P,i}}{u_i^2} (e^{-u_i} - 1 + u_i)$$

v_i ; molar volume, ϕ_i ; volume fraction,

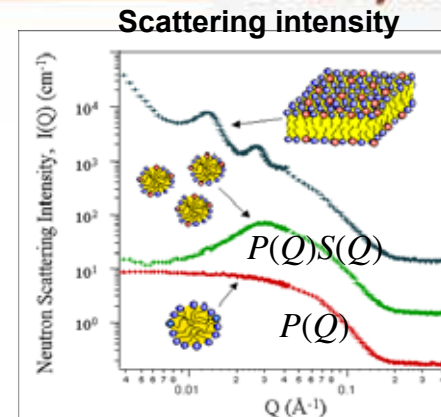
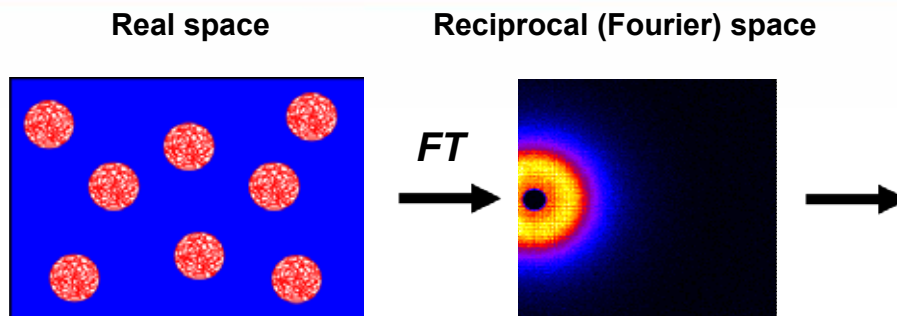
$$\frac{d\Sigma}{d\Omega} = (\beta_A - \beta_B)^2 v_0 S(Q)$$

$$\rightarrow Z_A, Z_B, R_{g,A}, R_{g,B}, \chi$$



Concentrated system (interacting system)

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Scattering intensity = Fourier transform of $|\text{contrast}|^2$

Absolute Scattering intensity

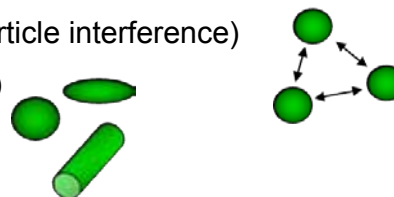
$$\frac{d\Sigma}{d\Omega} = \frac{N}{V} P(Q) S(Q) + I_{bg}$$

Number density (number of particles in cm^3)

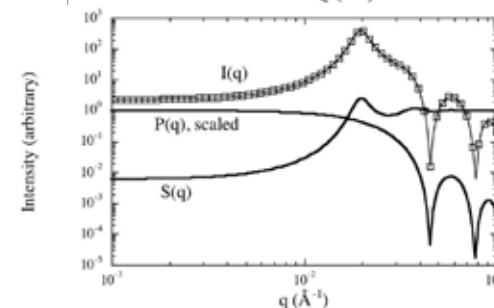
From factor (intra-particle interference)

Structure factor (inter-particle interference)

Background (due to incoherent scattering of H)



Scattering intensity is a product of Form and Structure factors.



Inter-particle interferences

Shibayama, CROSS

Scattering intensity

$$\frac{d\Sigma}{d\Omega} = \frac{N}{V}P(Q)S(Q) + I_{bg}$$

Structure factor

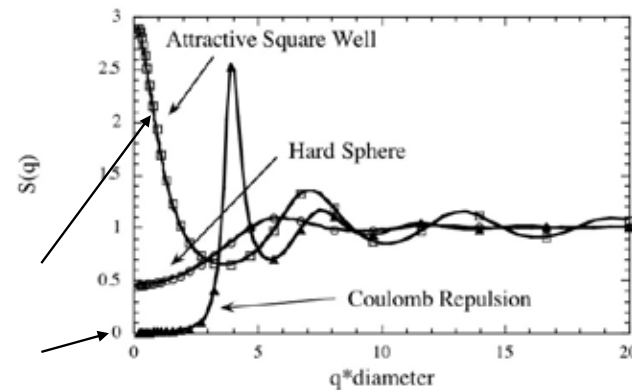
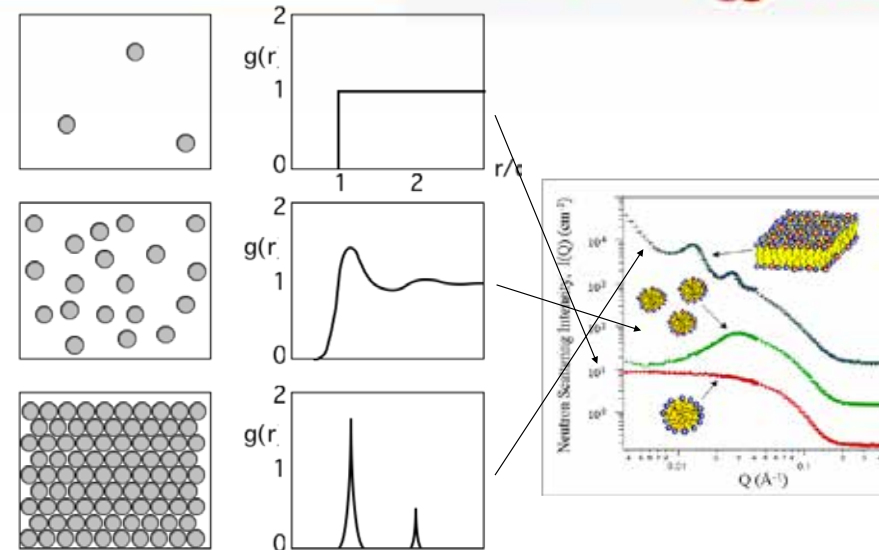
$$S(Q) = 1 + 4\pi n_p \int_0^\infty [g(r) - 1] \frac{\sin Qr}{Qr} r^2 dr$$

The low Q limit is proportional to the osmotic compressibility.

$$S(0) = k_B T \left(\frac{dn}{d\Pi} \right)$$

Attractive interaction -> more compressible

Repulsive interaction -> more compressible



Inter-particle interference fns.: $S(Q)$

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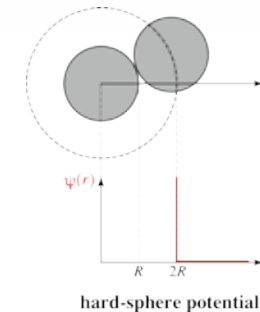
Various model $S(q)$ s are proposed, depending on the inter-particle potential function.

Debye (Hard sphere potential)

$$S_D(Q) = 1 - 8n_p V_p \Phi(2QR)$$

$$V_p = \frac{4\pi R^3}{3} \quad n_p: \text{the number density of spheres}$$

Interference peak appears by increasing number density, n_p !



Problem!: for the volume fraction $\phi_p = n_p V_p \geq 0.125$, $S_D(Q)$ becomes negative!

Other models of $S(Q)$

Fournet Avoiding the Debye fn. problem.

Percus-Yevick eq.

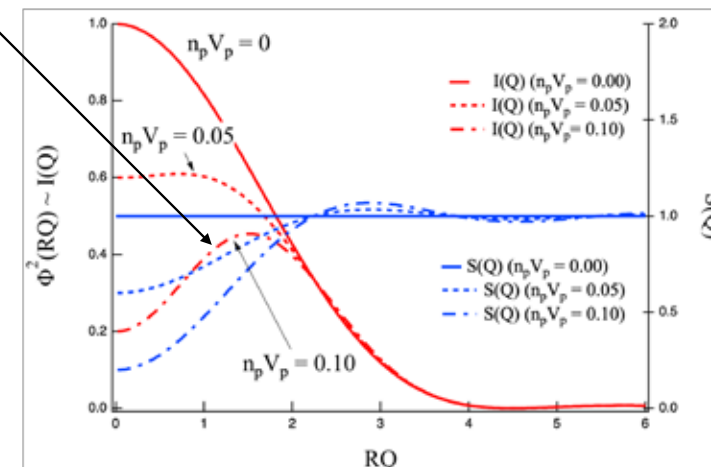
Considering direct correlation

Hayter-Penfold eq.

Macroion solutions

Freltoft-Kjems-Sinha eq.

Fractal aggregates



- (1) The SANS Toolbox, Boualem Hammouda (NIST)
- (2) Shibayama, in Neutron Scattering – Applications in Chemistry, Materials Science and Biology, pp. 459-546, Elsevier, 2017

Separation of $P(Q)$ and $S(Q)$ from $I(Q)$

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1. Observe $I(Q)$ s

$$I_{1,\text{obs}}(Q) \equiv \left(\frac{d\Sigma}{d\Omega}(Q) \right)_{1,\text{obs}} = \frac{N}{V} P(Q) + I_{bg} \quad (\text{dilute})$$

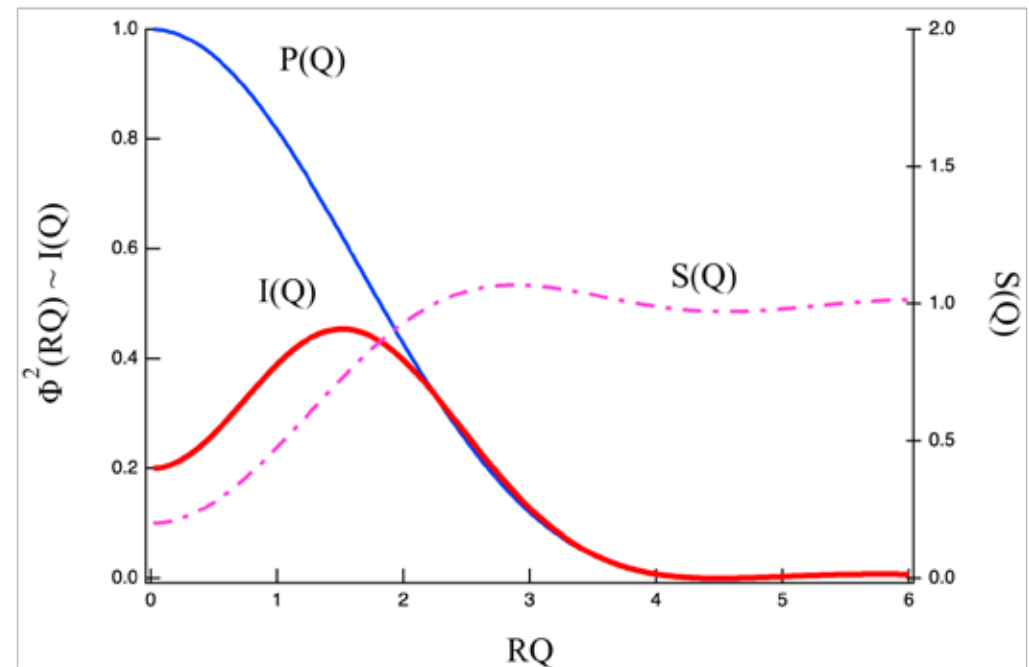
$$I_{2,\text{obs}}(Q) \equiv \left(\frac{d\Sigma}{d\Omega}(Q) \right)_{2,\text{obs}} = \frac{N}{V} P(Q) S(Q) + I_{bg} \quad (\text{finite conc.})$$

2. Subtract I_{bg}

Obtaining $P(Q)$

3. Divide $I_{2,\text{obs}}$ by $I_{1,\text{obs}}$

Obtaining $S(Q)$



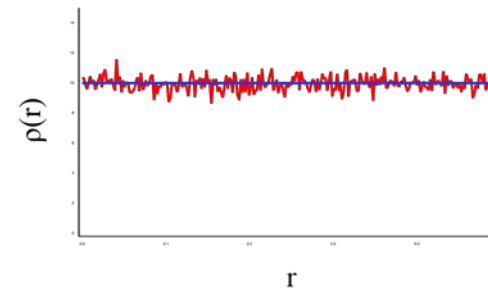
Scattering from fluctuating systems: Ornstein-Zernike fn.

Shibayama, CROSS

Ornstein-Zernike fn. is commonly used for describing **density (concentration) fluctuations in fluid systems**, magnetism, etc. (one phase system)

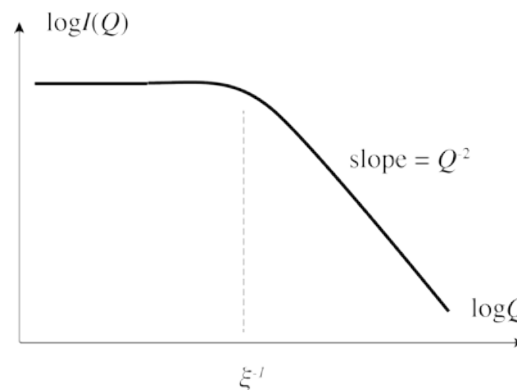
Correlation function (real space)

$$g(r) \propto \frac{\xi}{r} \exp\left(-\frac{r}{\xi}\right) \quad \text{Correlation length, } \xi$$

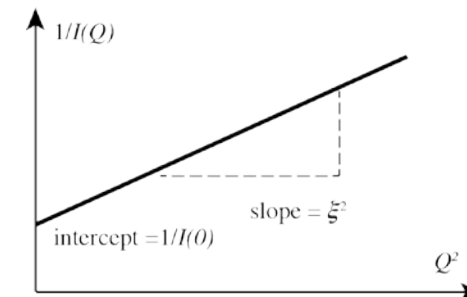


Ornstein-Zernike function (reciprocal space)

$$I(Q) = \frac{I(0)}{1 + \xi^2 Q^2}$$



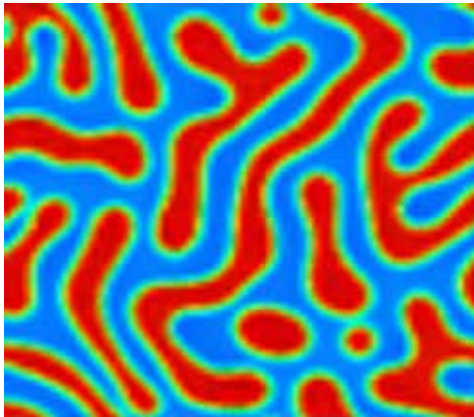
Ornstein-Zernike plot



Also applies to semi dilute polymer solutions, polymer gels, etc.

Non-particulate systems

Shibayama,  CROSS



Because of absence of concrete structural model
It is treated statistically with **the correlation function, $g(r)$** .

Correlation function (real space)

Scattering function (reciprocal space)

$$g(r) = \exp\left(-\frac{r}{\xi}\right)$$



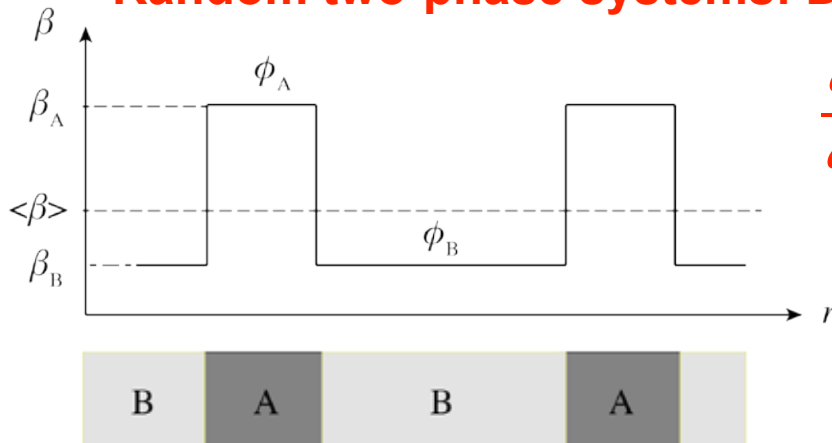
$$\frac{d\Sigma}{d\Omega}(Q) = 4\pi(\Delta\beta)^2 \int_V g(r) \frac{\sin(Qr)}{Qr} r^2 dr$$

Contrast

Orientation av.

Correlation fn.

Random two-phase systems: Debye-Buecke fn.



$$\frac{d\Sigma}{d\Omega}(Q) = 4\pi\langle\eta^2\rangle \int_V g(r) \frac{\sin(Qr)}{Qr} r^2 dr$$

$$\langle\beta\rangle = \phi_A\beta_A + \phi_B\beta_B$$

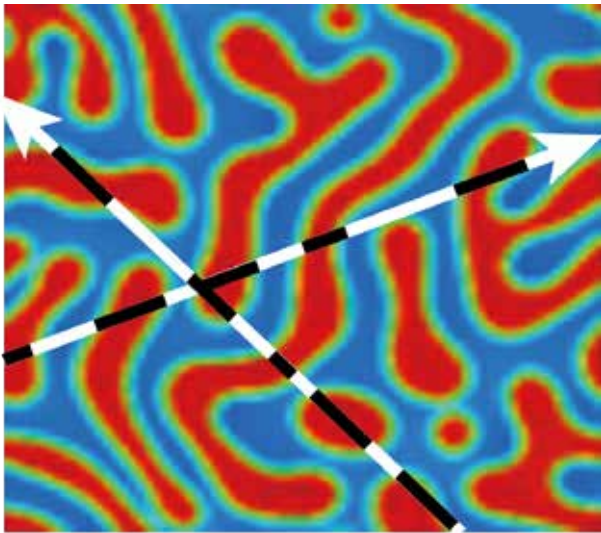
$$\eta_A = \beta_A - \langle\beta\rangle = (\beta_A - \beta_B)\phi_B = \Delta\beta\phi_B$$

$$\langle\eta^2\rangle = \phi_A\eta_A^2 + \phi_B\eta_B^2 = \phi_A\phi_B(\Delta\beta)^2$$

Random two-phase systems: Debye-Buecke fn.

Shibayama,  CROSS

For a two phase system with sharp boundary, **Debye-Bueche function** is often used, from which the size of island-sea structure is estimated.



$$I(Q) = \frac{I(0)}{(1 + \Xi^2 Q^2)^2}$$

Inhomogeneity length parameter, chord length

$$l_A = \frac{\Xi}{\phi_B}, l_B = \frac{\Xi}{\phi_A}$$

$$l = L_A + l_B = \left(\frac{1}{l_B} + \frac{1}{l_A} \right) \Xi$$

Babinet's principle

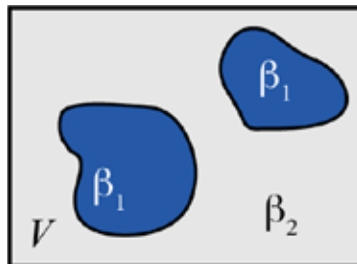
Shibayama, CROSS

Babinet's principle states that the diffraction pattern from an opaque body is identical to that from a hole of the same size and shape.

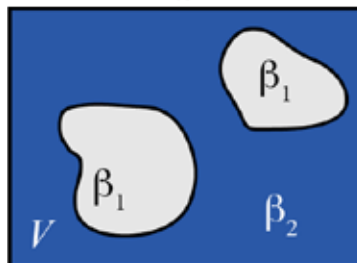
$$\begin{aligned}\frac{d\Sigma}{d\Omega}(Q) &= \frac{1}{V} \left| \int_{V_1} \beta_1 e^{i\mathbf{Q}\cdot\mathbf{r}} d^3r + \int_{V_2} \beta_2 e^{i\mathbf{Q}\cdot\mathbf{r}} d^3r \right|^2 \\ &= \frac{1}{V} (\beta_1 - \beta_2)^2 \left| \int_{V_1} e^{i\mathbf{Q}\cdot\mathbf{r}} d^3r \right|^2 = \frac{1}{V} (\beta_1 - \beta_2)^2 \left| \int_{V_2} e^{i\mathbf{Q}\cdot\mathbf{r}} d^3r \right|^2\end{aligned}$$



Jacques Babinet
Wikipedia



||



$$V = V_1 + V_2$$

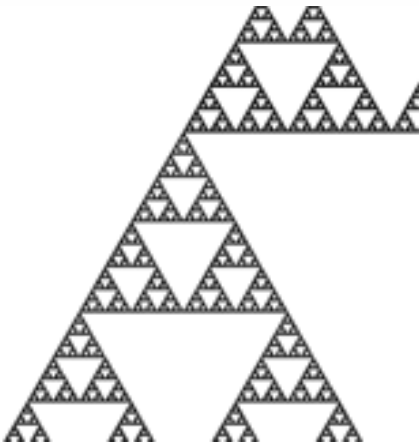
dependent only on
the difference of SLDs.

$$\frac{d\Sigma}{d\Omega}(Q) \propto (\beta_1 - \beta_2)^2$$

Q: Prove the Babinet's principle.

Scattering from Fractal objects

Shibayama, CROSS



Sierpinski zoom.gif

By I, Avenafatua, CC BY-SA 3.0,

<https://commons.wikimedia.org/w/index.php?curid=2304434>

Fractal: a shape or phenomenon that has self-similarity, looks similar even when enlarged or reduced

Found in; clusters, porous media, polymer chains, gelling system, etc.

mass fractal (fractal dimension; D)

$$\underset{\text{Mass}}{M} \sim \underset{\text{Size}}{R^D} \longleftrightarrow I(Q) \sim Q^{-D}$$

Ex. $I(Q) \sim Q^{-2}$

(Gaussian polymer chains)

surface fractal (fractal dimension; D_s)

$$\underset{\text{Total area}}{A_T} \sim \underset{\text{Size}}{R^{D_s}} \longleftrightarrow I(Q) \sim Q^{-(2d-D_s)}$$

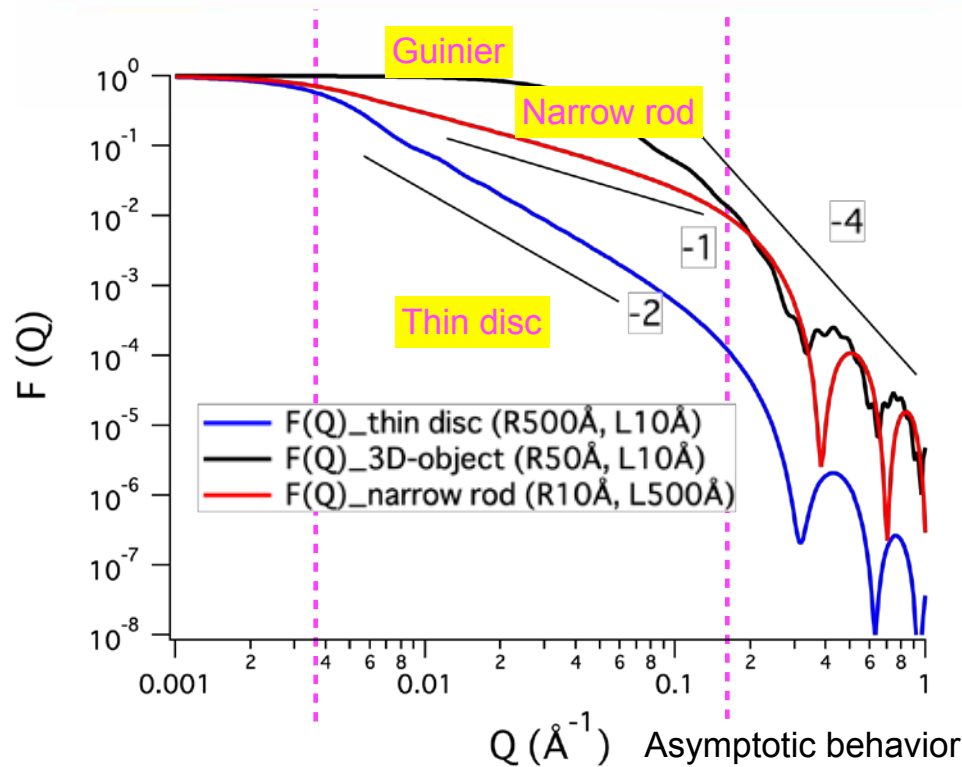
Ex. $I(Q) \sim Q^{-4}$

Space dimension: d

Two-phase system with smooth interface

Asymptotic Behavior

Shibayama, CROSS



	$Q_{x,1}$	$Q_{x,2}$
Thin disc	0	-2
Narrow rod	0	-1
3D obj.	0	-4

Two-phase system with smooth interface

$$I(Q) \sim Q^{-4} \quad \text{Porod law}$$

Fractal object (mass fractal)

$$I(Q) \sim Q^{-D}$$

Gaussian polymer chains ($D = 2$)

$$I(Q) \sim Q^{-2}$$

Fractal object (surface fractal)

$$I(Q) \sim Q^{-(2d-D_s)}$$

3d object with smooth surface ($d = 3, D_s = 2$)

$$I(Q) \sim Q^{-4} \quad \text{Porod law}$$

Unified equation: Beaucage (1995)

Shibayama, CROSS

Unified equation

$$I(Q) = G \exp\left(-\frac{R_g^2 Q^2}{3}\right) + B \left[\operatorname{erf}\left(\frac{R_g Q}{\sqrt{6}}\right)\right]^{3p} Q^{-p}$$

$$G = n^2 N_p I_e \quad B = 2\pi N_p \rho_e^2 S_p I_e = n^2 N_p I_e \cdot 2\pi \frac{S_p}{V_p^2}$$

n ; n . of electrons

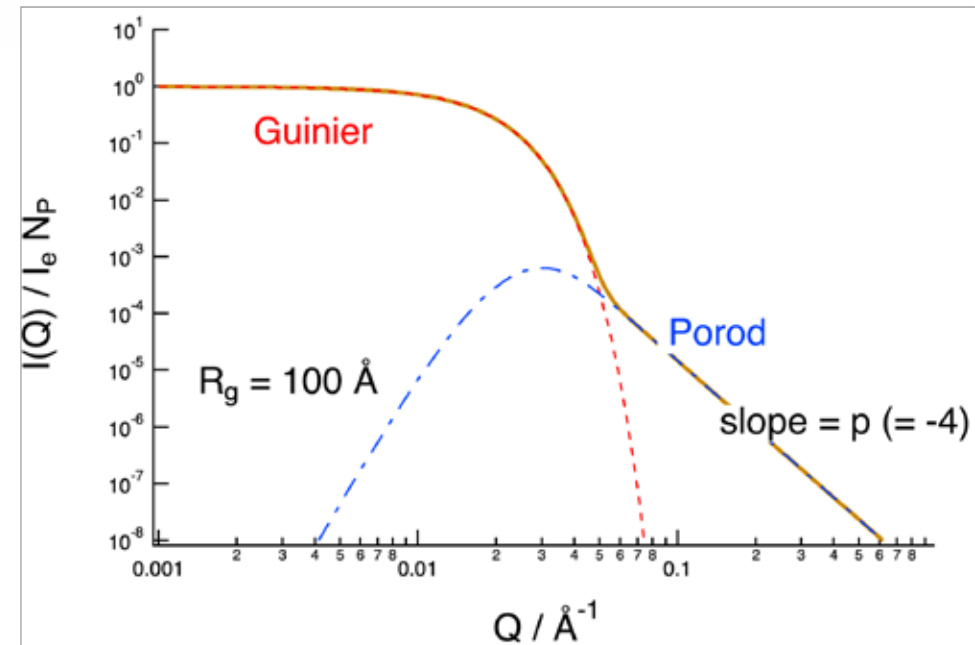
I_e ; scattering intensity of electron

N_p ; n . of particles

V_p, S_p ; volume/surface of particle

Multi-level of hierarchical structure

$$I(Q) = \sum_i \left\{ G_i \exp\left(-\frac{R_{g,i}^2 Q^2}{3}\right) + B_i \left[\operatorname{erf}\left(\frac{R_g Q}{\sqrt{6}}\right)\right]^{3p} Q^{-p} \right\}$$



Beaucage, G.

Approximations Leading to a Unified Exponential/Power-Law Approach to Small-Angle Scattering

J. Appl. Cryst., 1995, 28, 717-728

Summary (Part 3) : Various functions and plots in SAS

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Guinier function (dilute, low Q)

$$\ln I(Q) = \ln I(0) - \frac{R_g^2 Q^2}{3}$$

Information

Radius of gyration, R_g

Porod plot (two phase, large Q)

$$I(Q \rightarrow \infty) (\Delta\beta)^2 2\pi S_{sp} Q^{-4}$$

$$I(q) \propto Q^{-D}, \quad I(q) \propto Q^{-(6-D_s)}$$

$$I(q) \propto Q^{-4} \exp(-\sigma^2 Q^2)$$

Specific surface, S_{sp}

Mass fractal dimension, D

Surface fractal dimension, D_s

Interfacial thickness, t

$$\sigma = \sqrt{2\pi}t$$

Ornstein-Zernike function (one phase with fluctuations)

$$I(Q) = \frac{I(0)}{1 + \xi^2 Q^2}$$

Correlation length, ξ

Debye-Bueche function (two phase)

$$I(Q) = \frac{I(0)}{(1 + \Xi^2 Q^2)^2}$$

Inhomogeneity length parameter, Ξ

Chord length, l

$$l_A = \frac{\Xi}{\phi_B}, l_B = \frac{\Xi}{\phi_A} \quad l = L_A + l_B = \left(\frac{1}{l_B} + \frac{1}{l_A} \right) \Xi$$

Kratky plot (polymer solution)

$$Q^2 I(Q) \text{ vs } Q$$

Persistence length

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Analysis

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Q-space analysis

Grasping the overview of SANS functions,
(Rough analysis)

R_g (Guinier),
scattering exponent (Porod),
 Q_m (Scattering peak), etc.

r-space analysis

$$p(r) = \frac{1}{2\pi} \int_0^\infty I(Q) Q r \sin(Qr) dQ$$

Correlation fn.

Curve fitting with theoretical functions

(Detailed analysis)

Form factors (radius, etc.)
Structure factor (spacing, interaction, etc.)
Ornstein-Zernike (correlation length)
Debye-Bueche (chord length)
Kratky plot (chord length)
Debye function (polymer R_g)
Zimm plot ((polymer R_g , interaction parameter))
Random phase approximation (polymer R_g , interaction parameter)

Various corrections

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Shibayama et al., Macromol. Res., 2002, 74, S264.

Shibayama, CROSS

Particle-size distribution

$$I_R(q) = \langle n \rangle \Delta \rho^2 \frac{\int W(R) V^2(R) \Phi^2(qR) dR}{\int W(R) dR}$$

$$W_R(R) \sim \exp \left[-\frac{(R - \langle R \rangle)^2}{2\sigma_R^2} \right] \quad \langle n \rangle = \frac{w}{d_p \langle V \rangle} = \frac{\int W(R) dR}{\int W(R) V dR}$$

Wavelength distribution

$$I_{R+\lambda}(q) = \frac{w}{d_p} \Delta \rho^2 \frac{\int \int W_R(R) W_\lambda(\lambda) V^2(R) \Phi^2(qR) dR d\lambda}{\int \int W_R(R) W_\lambda(\lambda) V(R) dR d\lambda}$$

$$W_\lambda(\lambda) \sim \exp \left[-\frac{(\lambda - \langle \lambda \rangle)^2}{2\sigma_\lambda^2} \right] \quad \sigma_\lambda = \text{FWHM} / 2\sqrt{2 \ln 2}$$

$$\left(\frac{d\Sigma}{d\Omega} \right) = \frac{N}{V} (\beta_p - \beta_0)^2 \left(\frac{4\pi R^3}{3} \right)^2 \Phi^2(U) = \phi (\beta_p - \beta_0)^2 V_p \Phi^2(U)$$

$$U \equiv QR, \quad \Phi(U) \equiv \frac{3}{U^3} [\sin U - U \cos U]$$

$$\frac{N}{V} V_p^2 = \frac{N V_p}{V} V_p = \phi V_p$$

$$dq = -\frac{4\pi}{\lambda^2} \sin \theta d\lambda = -q \frac{d\lambda}{\lambda}$$

The effect of wavelength distribution becomes greater as q increases.

SANS analysis for polystyrene Beads in water

Shibayama, CROSS

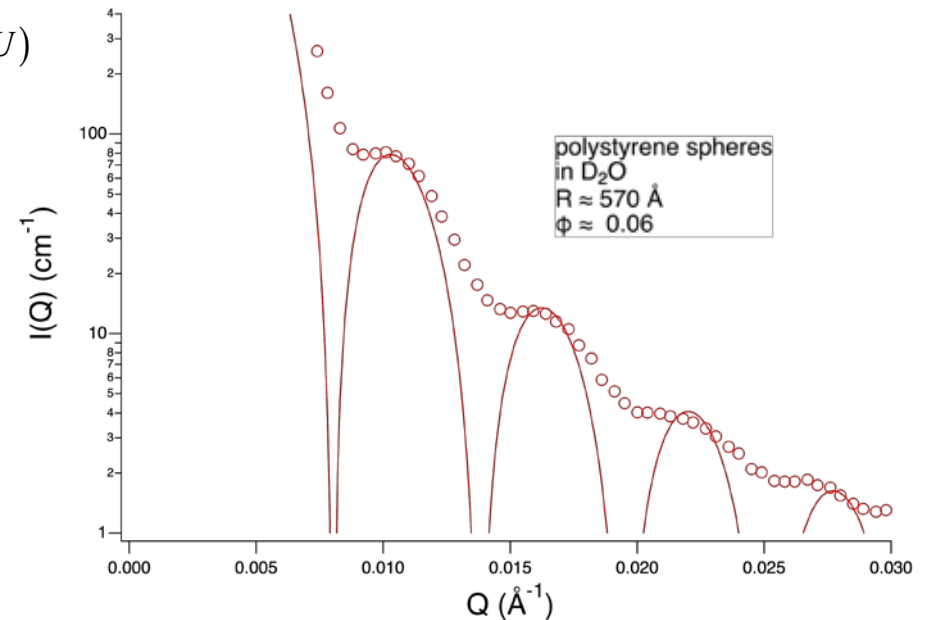
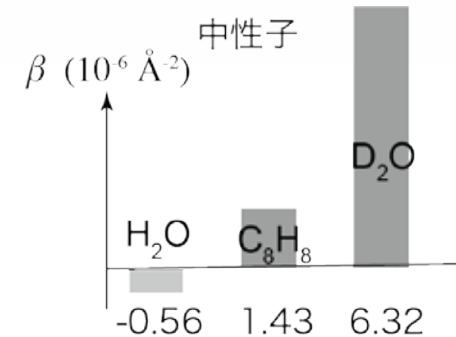
$$\left(\frac{d\Sigma}{d\Omega}\right) = \phi(\beta_p - \beta_0)^2 V_p \Phi^2(U) \quad [\beta_p = 1.43 \times 10^{10} \text{ cm}^{-2} (\text{C}_8\text{H}_8)]$$

$$U \equiv QR, \quad \Phi(U) \equiv \frac{3}{U^3} [\sin U - U \cos U] \quad [\beta_0 = 6.32 \times 10^{10} \text{ cm}^{-2} (\text{D}_2\text{O})]$$

$$\left(\frac{d\Sigma}{d\Omega}\right) = \phi(\beta_p - \beta_0)^2 V_p \Phi^2(U)$$

$$= 0.006 \times (1.43 \times 10^{10} - 6.32 \times 10^{10})^2 \times \frac{4\pi}{3} (560 \times 10^{-8})^3 \Phi^2(U)$$

$$= 10554 \times \Phi^2(U) [\text{cm}^{-1}]$$

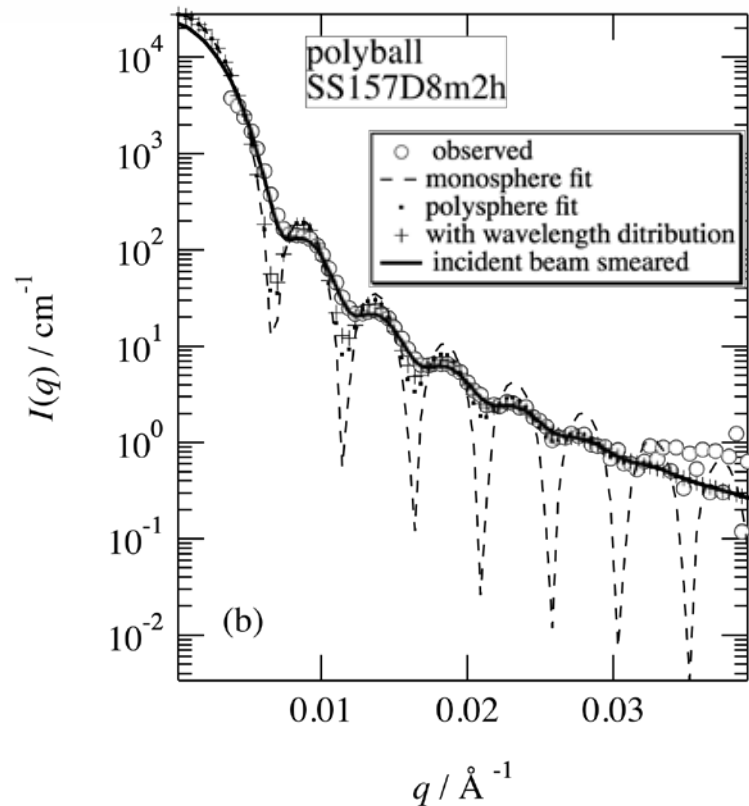


SANS of polystyrene beads in d-water

CUHK Lecture, M. Shibayama
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Shibayama et al., Macromol. Res., 2002, 74, S264.

Shibayama, CROSS



Fitting process:

- (1) sphere function (mono disperse)
- (2) Polydispersity
- (3) Wavelength distribution
- (4) Incident beam smearing

real-space analysis

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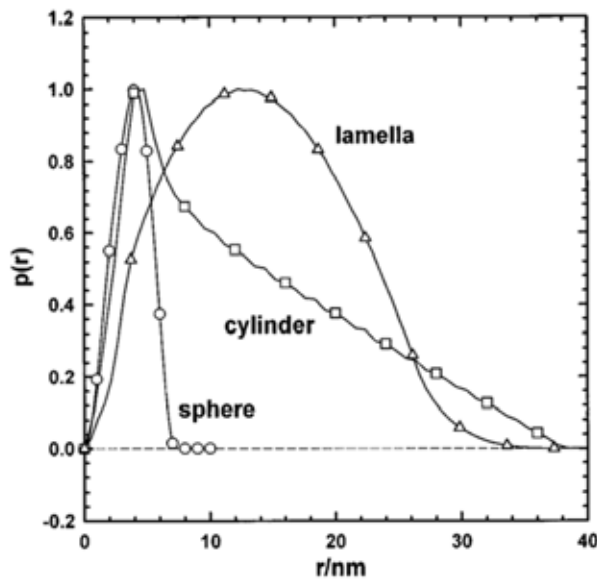
Strey, R., Glatter, O., Schubert, K.V., Kaler, E.W., Journal of Chemical Physics, 1996, 105, 1175-1188

Shibayama, CROSS

Indirect analysis (real space)

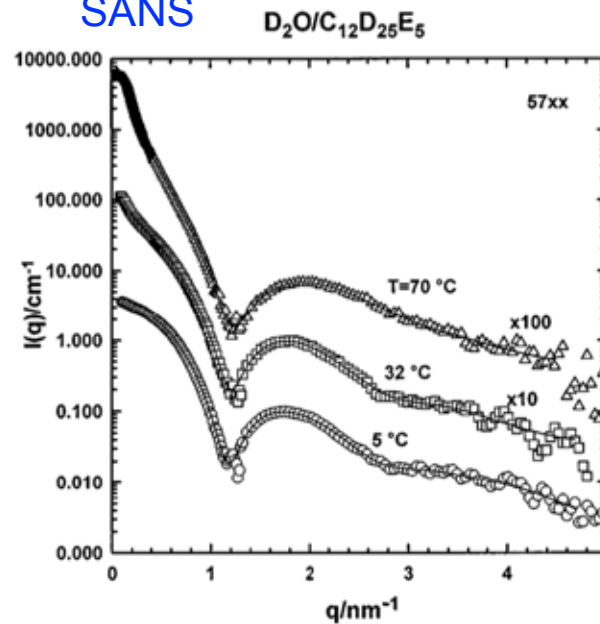
$$p(r) = \frac{1}{2\pi} \int_0^\infty I(Q) Q r \sin(Qr) dQ$$

Models

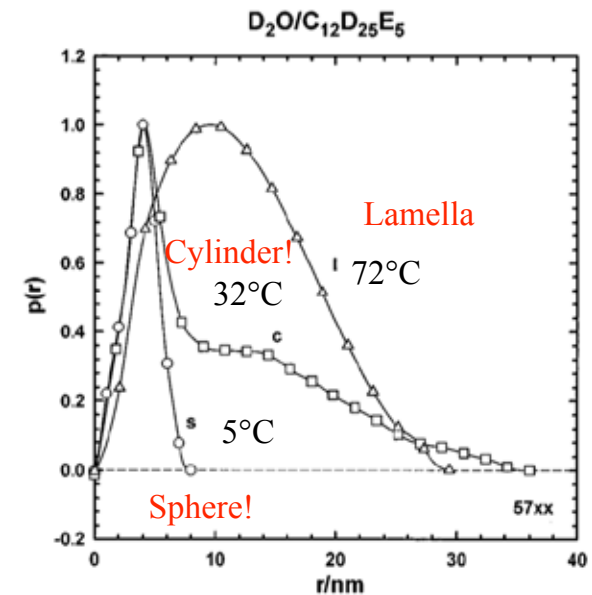


Hollow spheres,
Hollow cylinder,
Hollow lamella

SANS



r-space analysis



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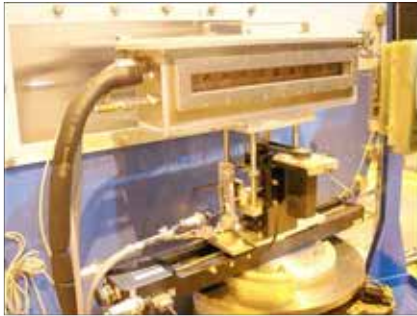
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Sample environments (SANS-U, ISSP)

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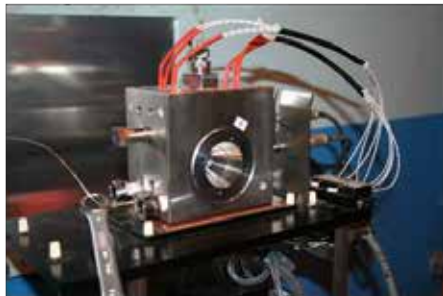
Default sample changer



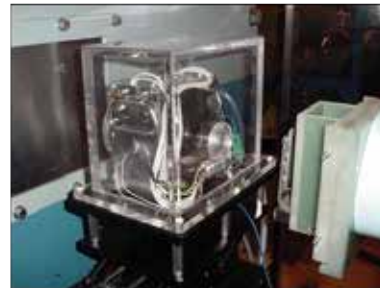
High-T cell



Stretching device



High-P cell (CO2)



High-P cell (~400MPa)



Flow cell (Rheo-SANS)

BL15 TAIKAN: sample environment

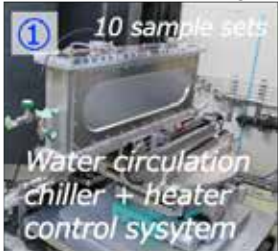
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For soft matter

Sample changer

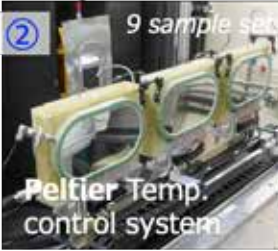
① 10 sample sets



Water circulation chiller + heater control system

$T = 5^{\circ}\text{C} - 180^{\circ}\text{C}$
(For high temp.)

② 9 sample sets

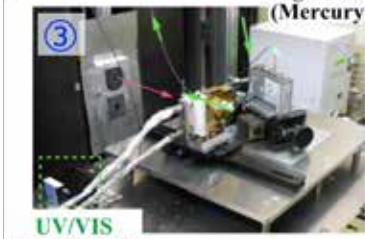


Peltier Temp. control system

$T = -20^{\circ}\text{C} - 80^{\circ}\text{C}$
(For low temp.)

Ultraviolet (UV) / visible (VIS) light control system

③



UV/VIS spectrometer

Light Source (Mercury Lamp)



80% humidity @ 80°C .

④ **Pressure cell**



$P_{\text{max}} : 50\text{MPa}$
 $T_{\text{max}} : 500^{\circ}\text{C}$

⑤ **Rheometer**
(Anton Paar :MCR302)



⑥ **Humidity gas generator**



Automatic control of gas ratios (H_2O and D_2O)

⑦ **humidity cell**



80% humidity @ 80°C .

⑧ **Sample changer with humidity chamber**



7 sample sets
80% humidity @ 80°C .

⑨ **Stretching machine with load cell**



For hard matter

Magnets

① 10T magnet with Laser heating furnace



② 4T magnet with Dilution refrigerator



$0.3\text{K} < T < 300\text{K}$

③ 1T magnet



④ 4K cryostat



⑤ Laser heating furnace



$T = \sim 1300\text{K}$

Rheo-SANS

Summary:

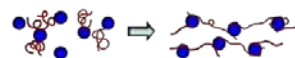
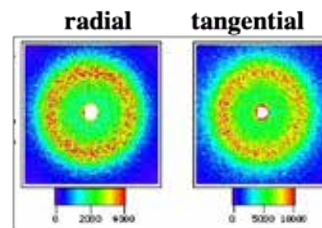
Rheo-SANS of Shear thickening

Rheometer for SANS



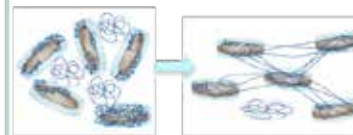
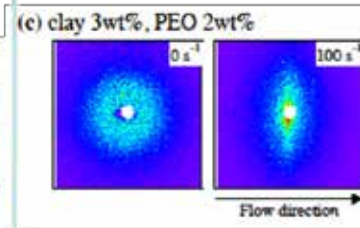
Simultaneous rheology and SANS measurements particle dispersion systems, gels, micelles, etc.

NE/HEC
Nanoemulsion/polymer



Shibayama et al.,
JCP, 2007, 127, 144507.

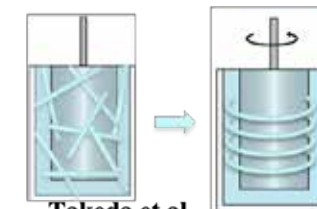
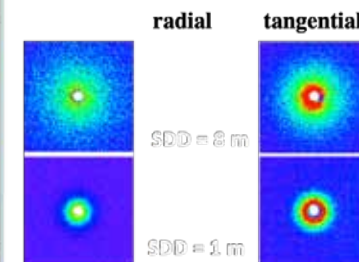
clay/PEO
Clay/polymer



Takeda et al.,
Macromolecules,
2010, 43, 7793.

Percolation transition

CTAB/NapTS
micelle

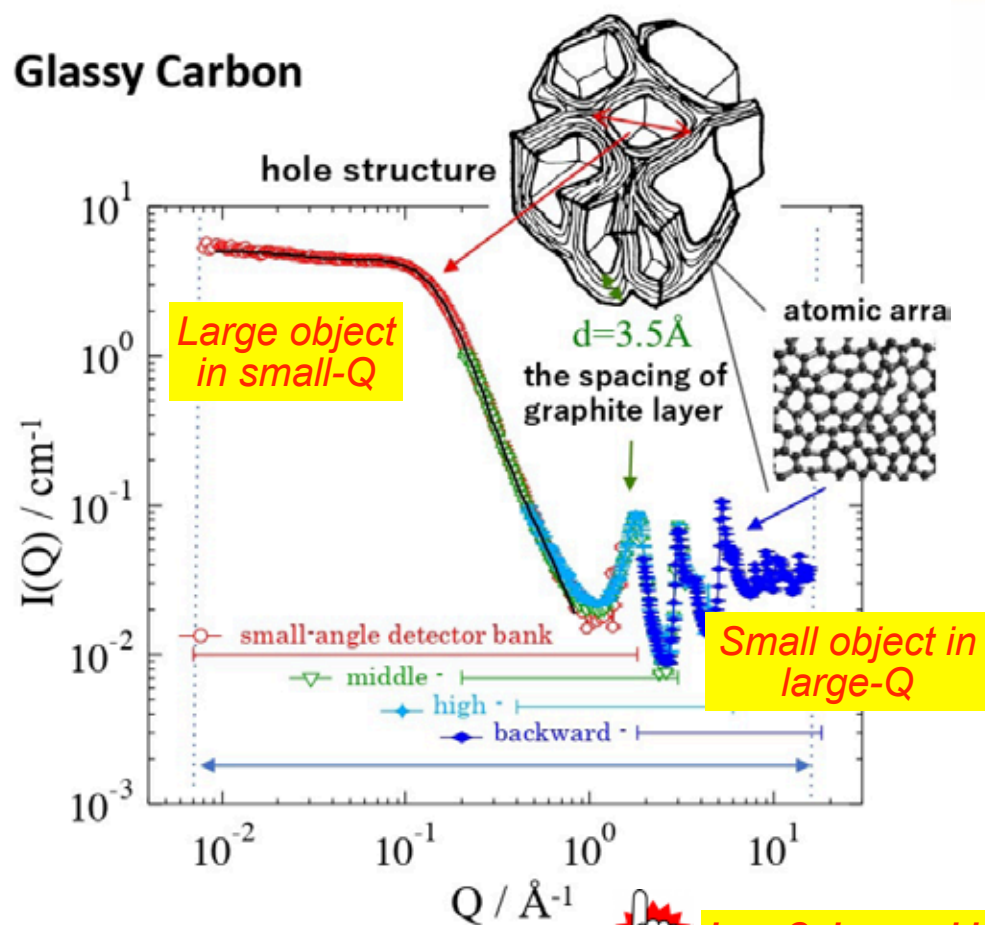


Takeda et al.,
Langmuir, 2011, 27, 1731.

Hierarchical structure of glassy carbon

Shibayama, CROSS

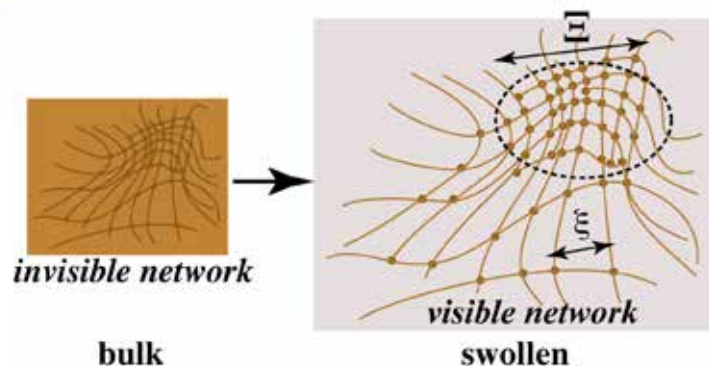
Glassy Carbon



Low-Q; Large objects, large-Q; small objects

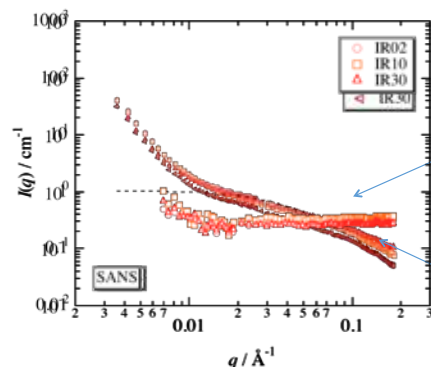
Visualization by D-solvent swelling

Shibayama, CROSS



 Invisible crosslink inhomogeneities
Can be visualized by D-solv.
Swelling.

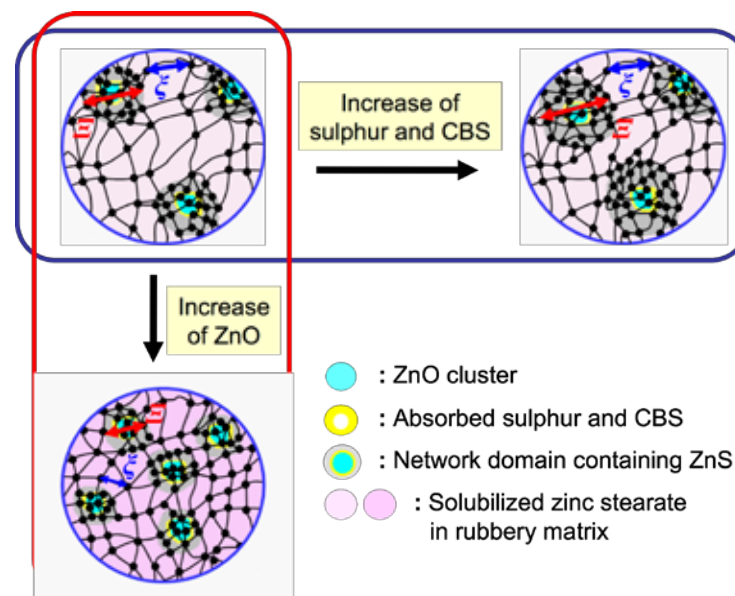
Biomacromolecules,
8, 693 (2007).
Macromolecules,
42, 2741 (2009)
Macromolecules,
43, 1556 (2010).



Bulk film

Swollen film

Suzuki, et al. Macromolecules 2010 43 1556



Vulcanization of natural rubber
Effects of zinc oxide (ZnO) and (CBS)(N-Cyclohexyl-2-benzothiazolyl sulfenamide)

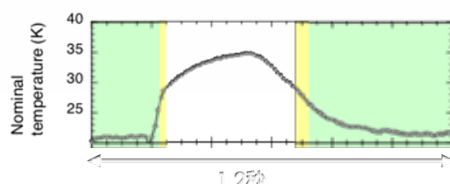
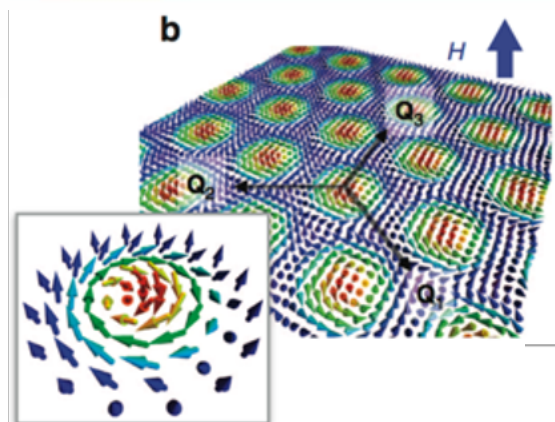
Repetitive measurement

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Nakajima, et al., Phys. Rev. B, 98, 014424 (2018)

Shibayama, CROSS

T. Nakajima, ISSP, UTokyo

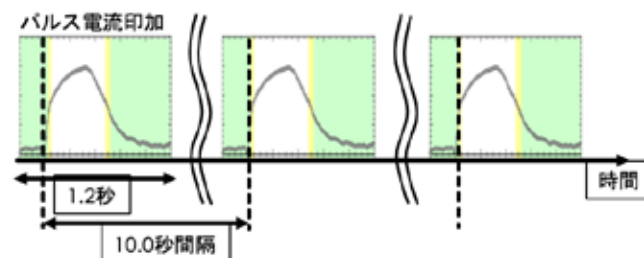


Direct observation
what happens
during temperature change.

Emergence of quasi-static skyrmion
by rapid heating/cooling

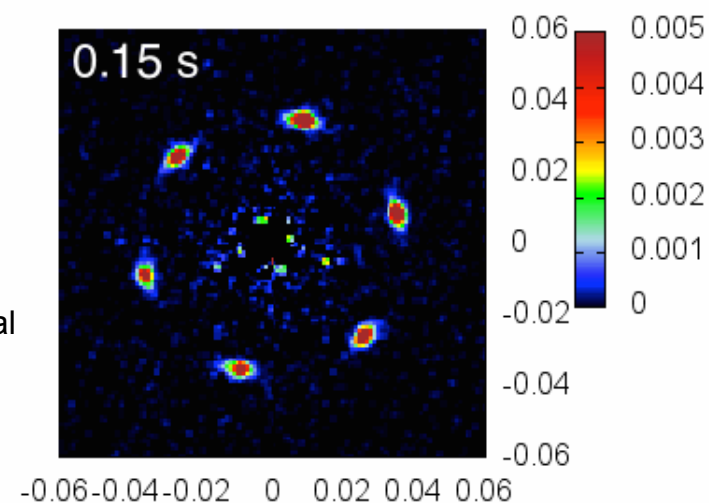
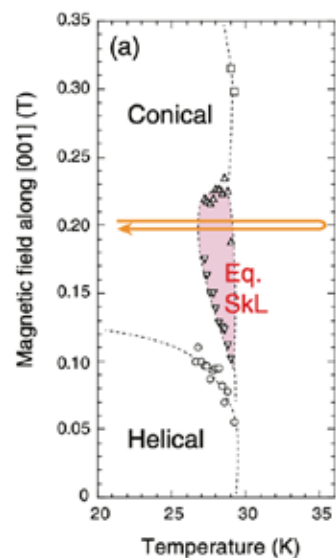
測定・解析手法

10Hz pulse electric current is imposed to the sample.



Repetitive collection of 1.2s-long data with 0.04s (25Hz) interval for 10s

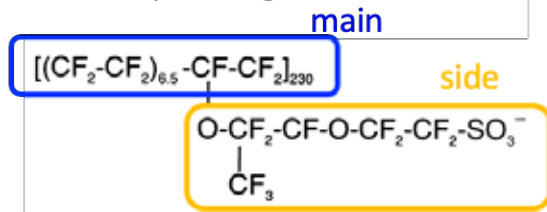
S/N can be improved by repetitive measurement even for weak scatterers.



Gas contrast variation with water vapor

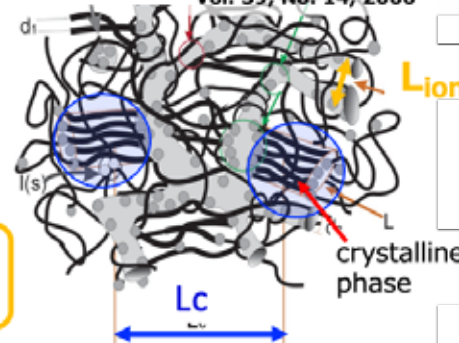
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Sample:
Nafion @ 117
prchased from Sigma-Aldrich
• thickness : 0.183 mm x 5
• density : 1.97 g/cm³

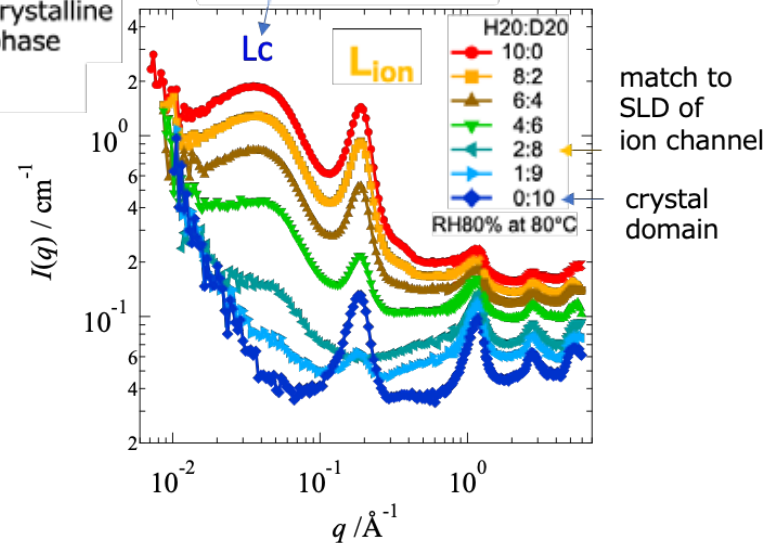
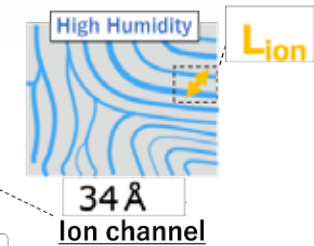
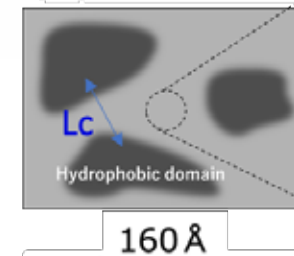


Structural model
of Nafion

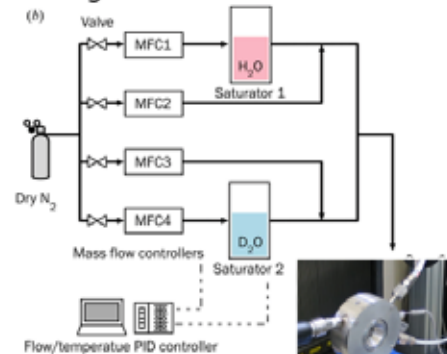
Kim et al. Macromolecules,
Vol. 39, No. 14, 2006



Correlation distance of
crystalline phases



Schematic of
the generator.



Automatic control of gas
ratios (H₂O and D₂O)

H/D humidity-controlled contrast-variation SANS

Sample environment: High-T, High-P cell for imaging

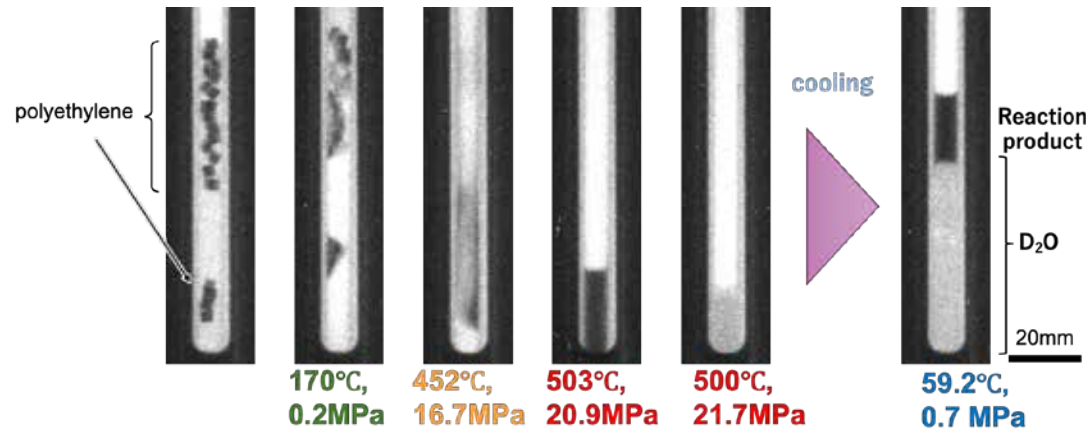
CUHK Lecture, M. Shibayama
2025.8.10 - 16

Abe, et al., Rev. Sci. Instrum. 94 083904 (2023).

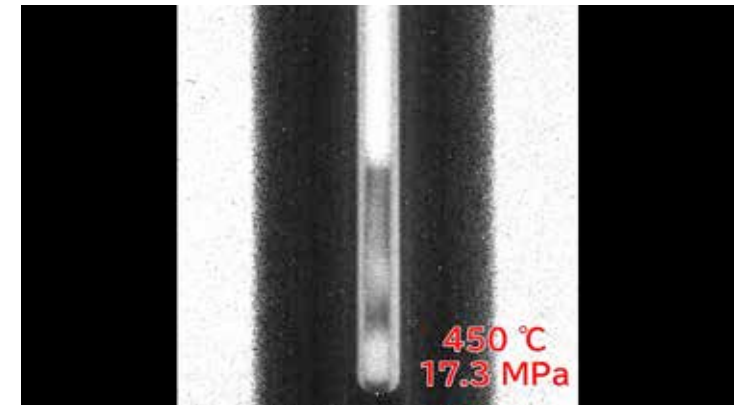
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Direct observation of polymer dissolution process in super-critical water

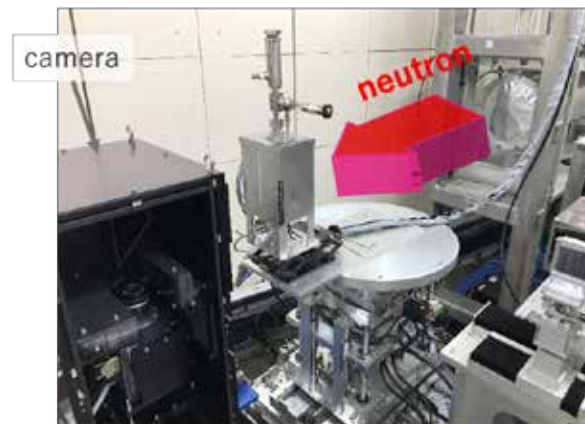
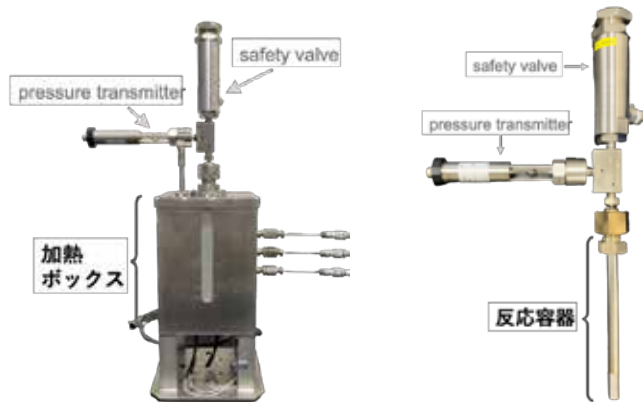
Neutron Imaging (TNRF; JRR-3)



PE pellets and D₂O



High T, high P cell



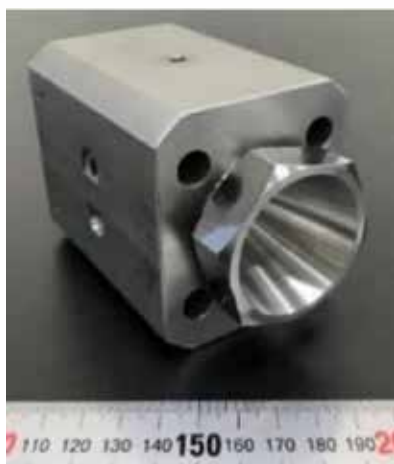
High-P safe sample environment

Abe et al., J. Appl. Cryst. (2024). 57, 306-313

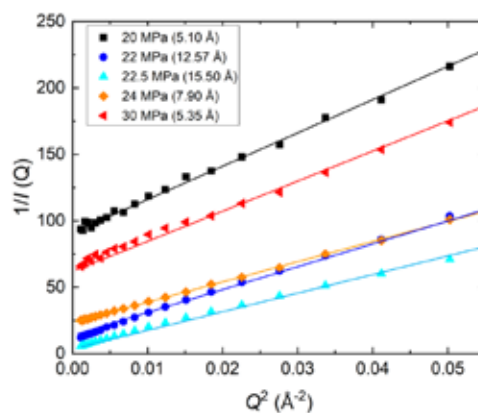
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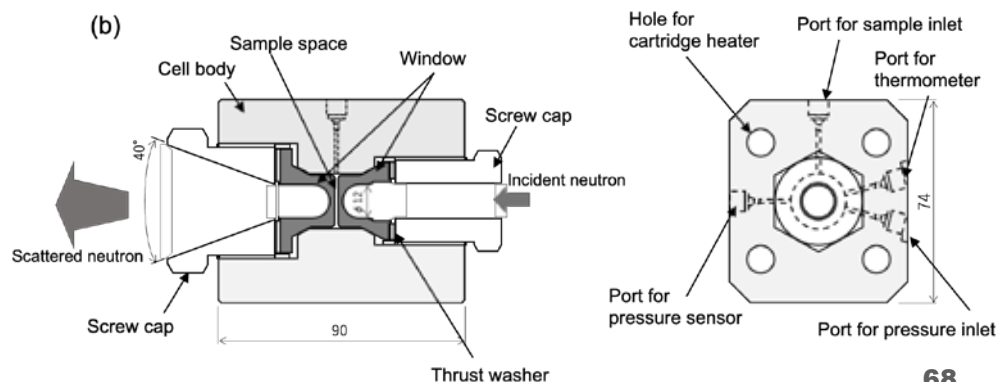
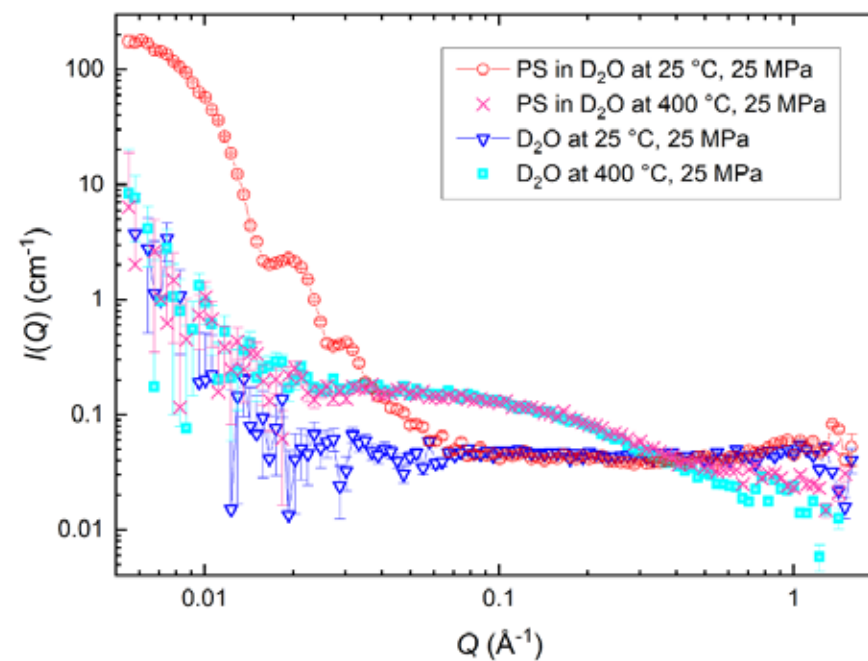
Ti alloy window with reasonable transmission, low parasitic scattering



$$\frac{1}{I(q)} = \frac{1}{I(0)} + \frac{\xi^2}{I(0)} q^2$$



Polystyrene particles in D₂O

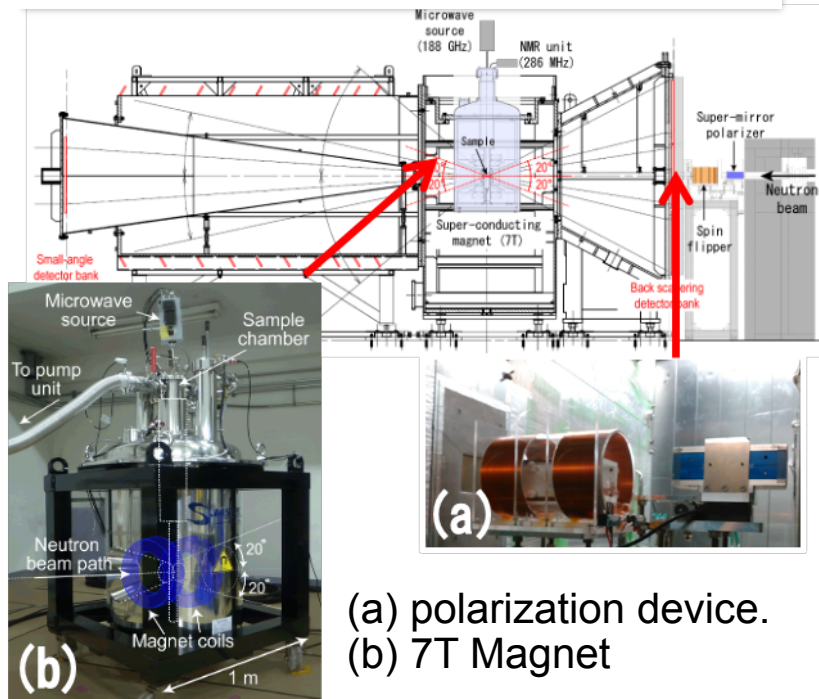


Dynamic Nuclear Polarization-SANS

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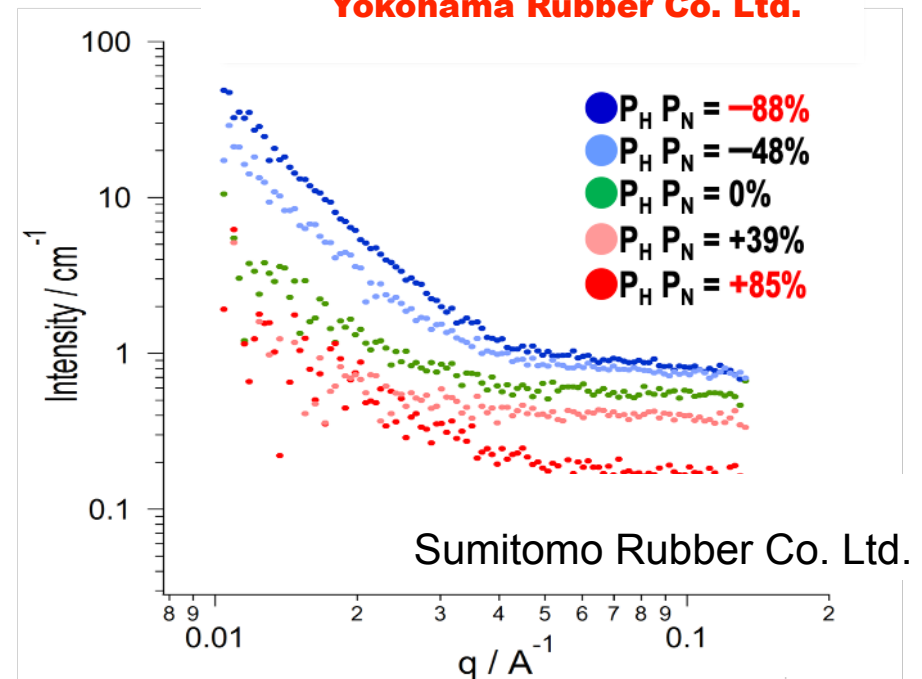
Dynamic Nuclear Polarization Small Angle Neutron Scattering

DNP-SANS setup@iMATERIA



DNP-SANS of SBR rubber

Yokohama Rubber Co. Ltd.



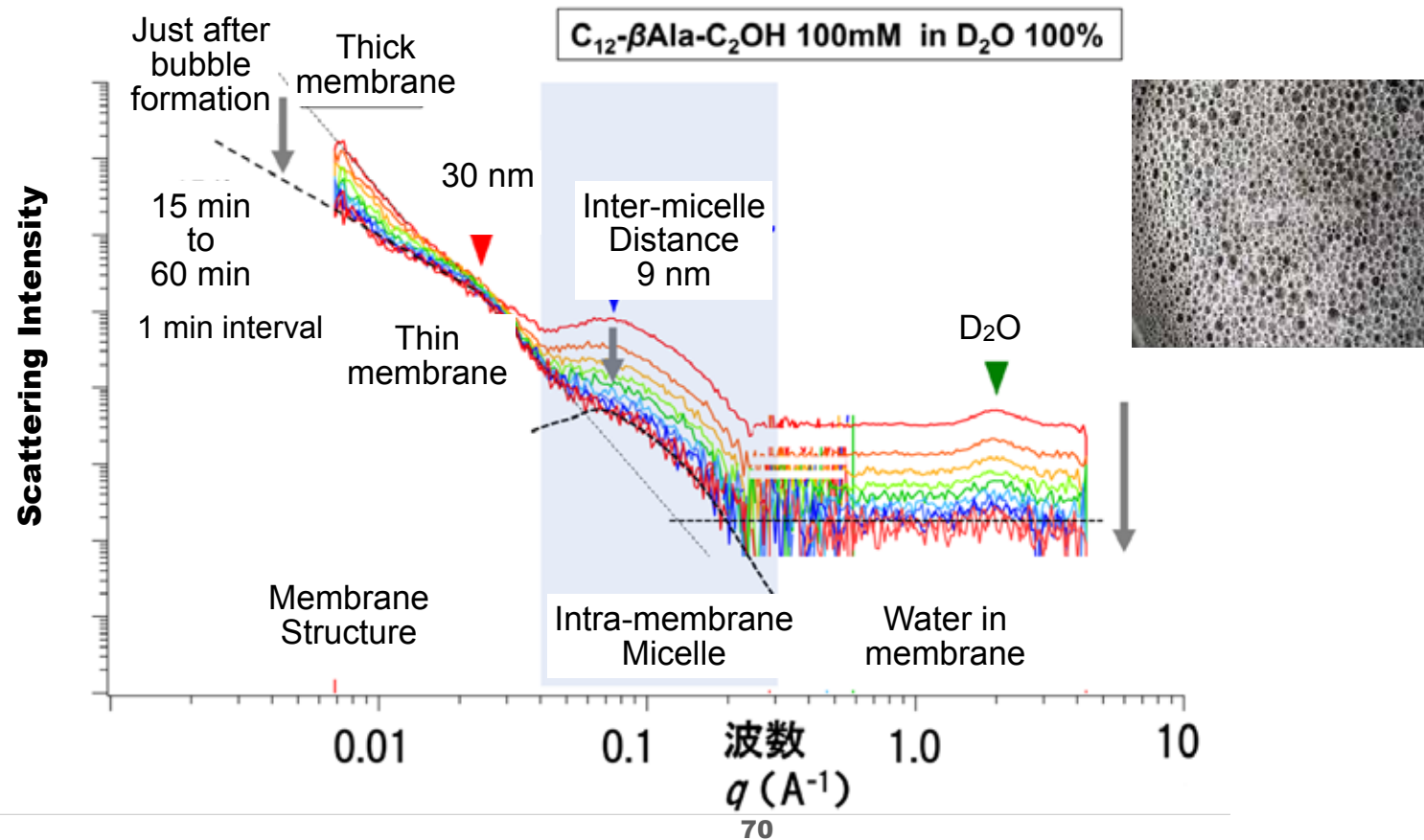
Time-resolved SANS

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Foam collapse process

NOF CORPORATION, Ibaraki U., Nara Womens U., Kracie, Ltd.



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Part 1. Overview:

1. SANS in Material sciences
2. SANS instruments
3. Angle dispersion vs TOF measurements

Part 2. Basics of Neutron scattering

Part 3. SANS theory

1. Guinier law
2. Form factors (sphere, cylinder, etc.)
3. Porod law
4. Polymer
5. Interacting systems
6. One-phase systems (Ornstein-Zernike)
7. Multi-phase systems (Debye-Bueche)
6. Fractals
8. Asymptotic behaviors

Part 4. Analysis

1. Q-space analysis
2. Corrections
3. real space analysis

Part 5. Applications and Topics

1. Sample environment
2. Topics

Part 6. Summary and reference

Summary

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Many materials, both natural and man-made, have sizes ranging from **a few nm to several tens of nm**. Small-angle neutron scattering (**SANS**) is an important tool for determining **the size and structure** of these materials.

Principles, features, and theoretical overview of neutron scattering are given in this lecture.

I hope that you will take this opportunity to consider and conduct small-angle neutron scattering experiments at large facilities such as **CSNS, and J-PARC MLF**.

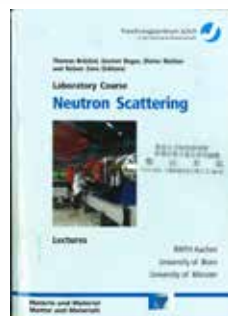
Contents and Ref. Books

Shibayama,  CROSS

(1) Higgins,
1994



(2) Brückel, 2005



(3) Sivia, 2011



(4) Shibayama,
2017



(5) Hashimoto
2022



(6) Shibayama
2025



References:

- (1) J. S. Higgins, H. C. Benoit, Polymers and Neutron Scattering, Oxford Press, 1994.
- (2) T. Brückel, et al., Neutron Scattering, Jülich, 2005
- (3) D.S. Sivia, Elementary Scattering Theory for X-ray and Neutron Users, Oxford, 2011.
- (4) M. Shibayama, Soft Condensed Matter, in “Neutron Scattering – Applications in Chemistry, Materials Science and Biology”, Fernandez-Alonso, F. and Price, D. L. Eds., 2017
- (5) T. Hashimoto, Principles and Applications of X-ray, Light and Neutron Scattering, Springer, 2022.
- (6) M. Shibayama, Introduction to Neutron Scattering, Kodansha, 2025. (Jpn)

(0) B. Hammouda, The SANS Toolbox (NIST)

https://www.eng.uc.edu/~beaucag/Courses/Properties/the_SANS_toolbox.pdf

Useful reference: Hammouda's SANS Toolbox

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PROBING NANOSCALE STRUCTURES – THE SANS TOOLBOX
B. Hammouda, NIST, 2016

https://www.eng.uc.edu/~beaucag/Classes/Properties/the_SANS_toolbox.pdf

http://www.ncnr.nist.gov/staff/hammouda/the_SANS_toolbox.pdf

A tutorial review of SANS, covering neutron sources, basic theory, instrumentation, data correction and reduction, modeling, and examples of a variety of systems, including polymers, complex fluids, and biological systems.

