Methoden moderner Röntgenphysik: Streuung und Abbildung

Lecture 6	Vorlesung zum Haupt- oder Masterstudiengang Physik, SoSe 2021		
	G. Grübel, O. Seeck, V. Markmann, F. Lehmkühler, Andre Philippi-Kobs, M. Martins		
Location	online		
Date	Tuesdays	12:30 - 14:00	(starting 6.4.)
	Thursdays	8:30 - 10:00	(until 8.7.)

Methoden moderner Röntgenphysik: Online Info

Tuesday Zoom-Meeting
https://desy.zoom.us/j/92674682486
Meeting ID: 926 7468 2486
Passcode: 144456

Thursday Zoom-Meeting
https://desy.zoom.us/j/99738625981
Meeting ID: 997 3862 5981
Passcode: 841881

Tutorial Zoom-Meeting
https://desy.zoom.us/j/95288979489
Meeting ID: 952 8897 9489
Passcode: 832350

Literature

Basic concepts:

Moderne Röntgenbeugung
Röntgendiffraktometrie für Materialwissenschaftler, Physiker und Chemiker
Authors
(view affiliations)
Lothar Spieß
Robert Schwarzer
Herfried Behnken
Gerd Teichert
https://link.springer.com/book/10.1007/978-3-663-10831-3

Elements of Modern X-Ray Physics
J. A. Nielsen and D. McMorrow, J. Wiley&Sons (2001)

X-Ray Diffraction
B.E. Warren, DOVER Publications Inc., New York

Principles of Optics
M. Born and E. Wolf, Cambridge University Press, 7th ed.

Soft X-rays and Extreme Ultraviolet Radiation
D. Attwood, Cambridge University Press (2000)
http://www.coe.berkeley.edu/AST/sxreuv/

Physik der Teilchenbeschleuniger und Synchrotronstrahlungsquellen
K. Wille, Teubner Studienbücher 1996

Lecture Notes

https://photon-science.desy.de/research/research_teams/coherent_x_ray_scattering/teaching/index_eng.html

Methoden moderner Röntgenphysik: Streuung und Abbildung

Part I:

Basics of X-ray Physics

by Gerhard Grübel (GG)

Introduction
Overview, Introduction to X-ray Scattering

X-ray Scattering Primer & Sources of X-rays +Synchrotron Radiation
Elements of X-ray Scattering, Laboratory Sources, Accelerator Bases Sources

Reflection and Refraction from Interfaces
Snell's Law, Fresnel Equations

Kinematical Diffraction (I)
Diffraction from an Atom, a Molecule, from Liquids, Glasses, …

Kinematical Diffraction (II)
Diffraction from a Crystal, Reciprocal Lattice, Structure Factor, …

Methoden moderner Röntgenphysik: Streuung und Abbildung

Small Angle Scattering, and Soft Matter
Introduction, Form Factor, Structure Factor, Applications, ...

Anomalous Diffraction
Introduction into Anomalous Scattering, ...

Introduction into Coherence
Concept, First Order Coherence, Spatial Coherence, Second Order Coherence, ...

Coherent Scattering
Imaging and Correlation Spectroscopy, ...

The Liquid Structure Factor

Consider mono-atomic or mono-molecular systems:

$$I(\mathbf{Q}) = f(\mathbf{Q})^2 \, {}_n\Sigma \, e^{i\mathbf{Q}\mathbf{r}_n} \, {}_m\Sigma \, e^{i\mathbf{Q}\mathbf{r}_m} = f(\mathbf{Q})^2 \, {}_n\Sigma_m\Sigma \, e^{i\mathbf{Q}(\mathbf{r}_n - \mathbf{r}_m)}$$

with f(**Q**) form factor

separate summations

$$I(\mathbf{Q}) = Nf(\mathbf{Q})^2 + f(\mathbf{Q})^2 \, {}_{n,\,m}\Sigma_{m\neq n}\Sigma \, e^{i\mathbf{Q}(\mathbf{r}_n - \mathbf{r}_m)}$$

Replace m≠n sum by integral and separate out average density ρ_{at}:

$$I(\mathbf{Q}) = \underline{Nf(\mathbf{Q})^2 + f(\mathbf{Q})^2 \, {}_n\Sigma \, {}_V\!\int [\rho_n(\mathbf{r}_{nm}) - \rho_{at}] \, e^{i\mathbf{Q}(\mathbf{r}_n - \mathbf{r}_m)}} dV_m + \underline{f(\mathbf{Q})^2 \, \rho_{at} \, {}_n\Sigma \, {}_V\!\int e^{i\mathbf{Q}(\mathbf{r}_n - \mathbf{r}_m)} dV_m}$$

I_{SRO} (Q)

measures short-range order (SRO) since

$\rho_n(\mathbf{r}_{nm}) \rightarrow \rho_{at}$ after few atomic spacings

and the term oscillates then towards zero

I_{SAXS} (Q)

contributes only for Q → 0

(otherwise oscillates to zero)

where $\rho_n(\mathbf{r}_{nm})\, dV_m$ is the number of atoms in element dV_m located at $\mathbf{r}_m$ - $\mathbf{r}_n$ relative to $\mathbf{r}_n$.

Small Angle X-ray Scattering (SAXS)

From Eq. (**)

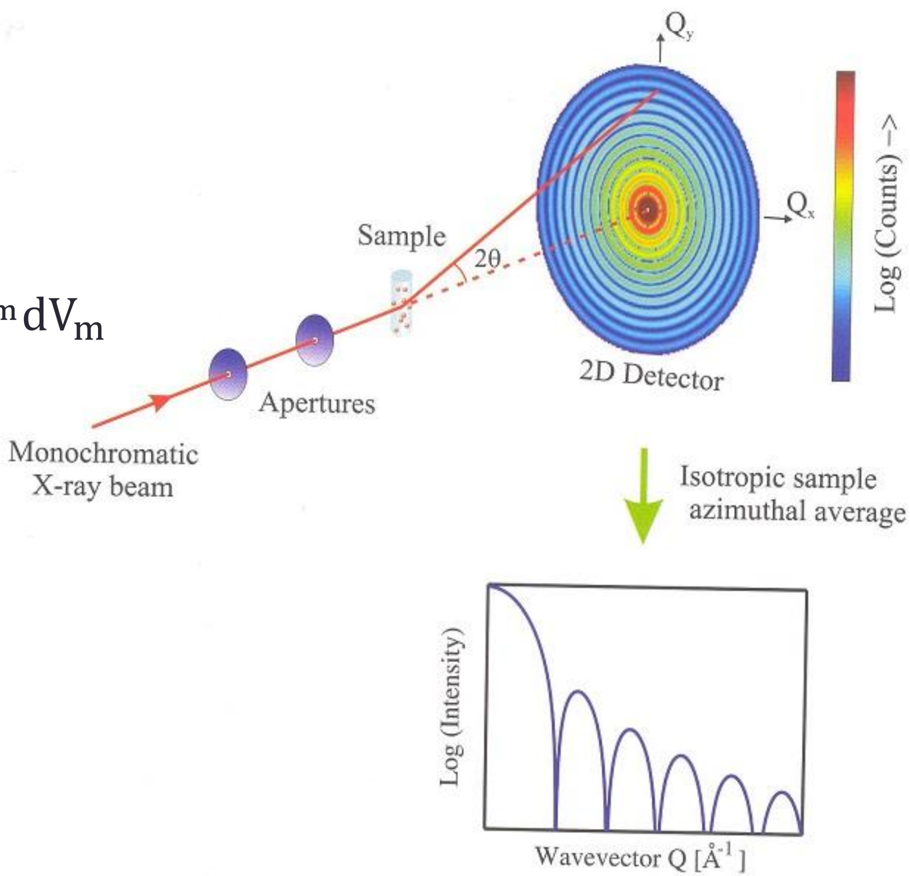
$$I_{SAXS}(Q) = f^2 \sum_n \int_V \rho_{at}\, e^{i\mathbf{Q}(\mathbf{r}_n-\mathbf{r}_m)} dV_m$$

$$= f^2 \sum_n e^{i\mathbf{Q}\mathbf{r}_n} \int_V \rho_{at}\, e^{-i\mathbf{Q}\mathbf{r}_m}\, dV_m$$

$$= f^2 \int_V \rho_{at}\, e^{i\mathbf{Q}\mathbf{r}_n} dV_n \int_V \rho_{at}\, e^{-i\mathbf{Q}\mathbf{r}_m} dV_m$$

$$\Rightarrow I_{SAXS}(Q) = \left| \int_V \rho_{sl}\, e^{i\mathbf{Q}\mathbf{r}} dV \right|^2$$

with $\rho_{sl} = f\,\rho_{at}$



SAXS (Form Factor)

The form factor of isolated particles

$$I_{SAXS}(Q) = \left(\rho_{sl,p} - \rho_{sl,0}\right)^2 \left| \int_{Vp} e^{iQr} dV_p \right|^2$$

Where $\rho_{sl,p}$, $\rho_{sl,0}$ are the scattering length densities of the particle (p) and solvent (0) and V_p is the volume of the particle.

Using the particle form factor $$F(Q) = \frac{1}{V_p} \int_{Vp} e^{iQr} dV_p$$

one finds $I_{SAXS}(Q) = \Delta\rho 2\ V^2{}_p\ |F(Q)|2$ with $\Delta\rho = \rho_{sl,p} - \rho_{sl,0}$

The form factor depends on the morphology (size and shape of the particles) and can be evaluated analytically only in a few cases:

For a sphere with radius R one finds:

$$F(Q) = \frac{1}{V_p} \int_0^R \int_0^{2\pi} \int_0^{\pi} e^{iQr\cos(\theta)}\, r^2 \sin\theta\, d\theta d\phi dr = \frac{1}{V_p} \int_0^R 4\pi \frac{\sin(Qr)}{Qr} r^2 dr$$

$$= 3\frac{\sin(QR) - Qr\cos(QR)}{(QR)^3} = 3\frac{J_1(QR)}{QR}$$

with $J_1(x)$: Bessel function of the first kind.

For $Q \rightarrow 0$: $|F(Q)|^2 = 1$ and $I_{SAXS}(Q) = = \Delta\rho^2\ V^2{}_p$

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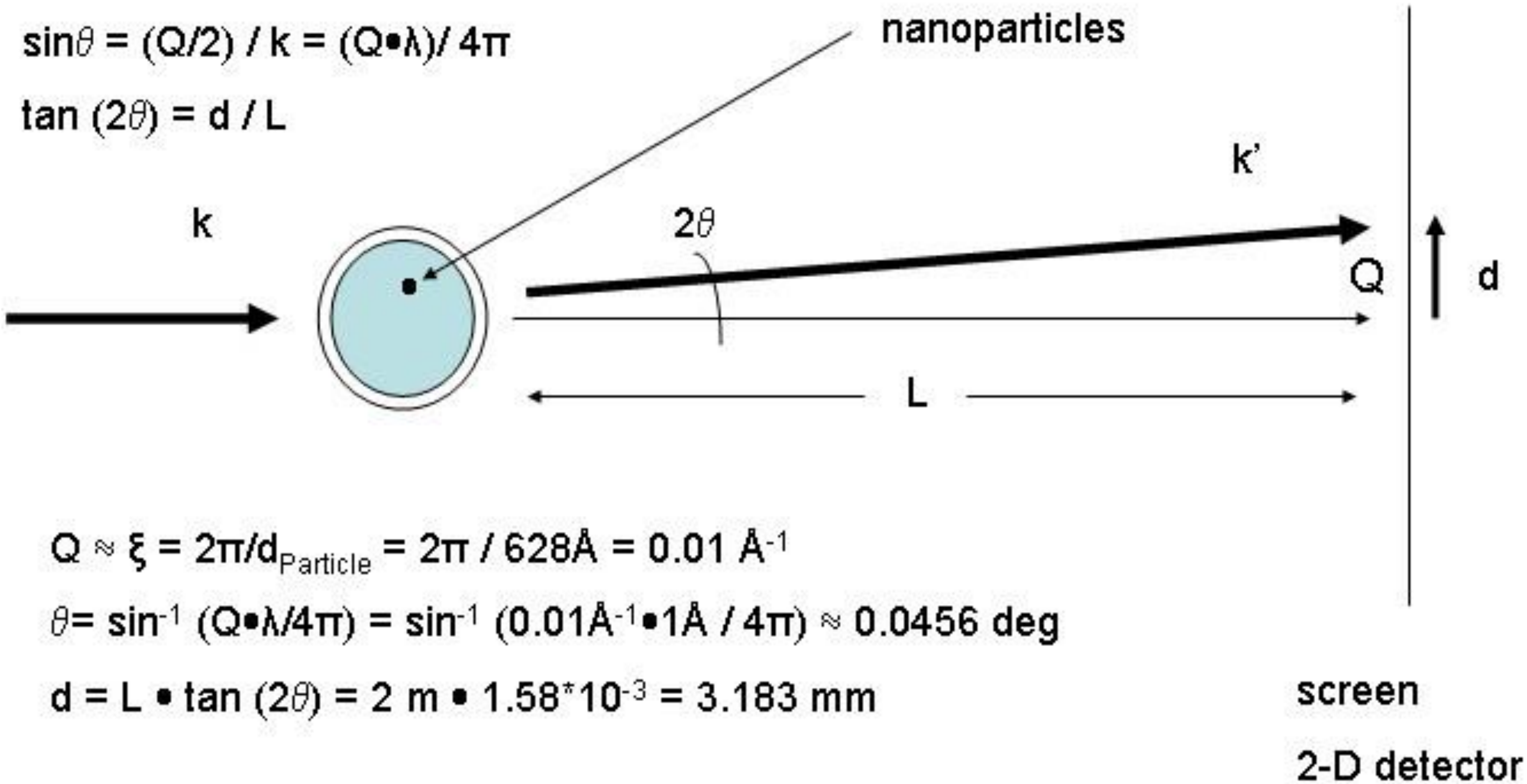
Experimental Set-up (SAXS)

Consider objects (nano-structures) of sub-µm size

$\sin\theta = (Q/2) / k = (Q \bullet \lambda) / 4\pi$

$\tan(2\theta) = d / L$



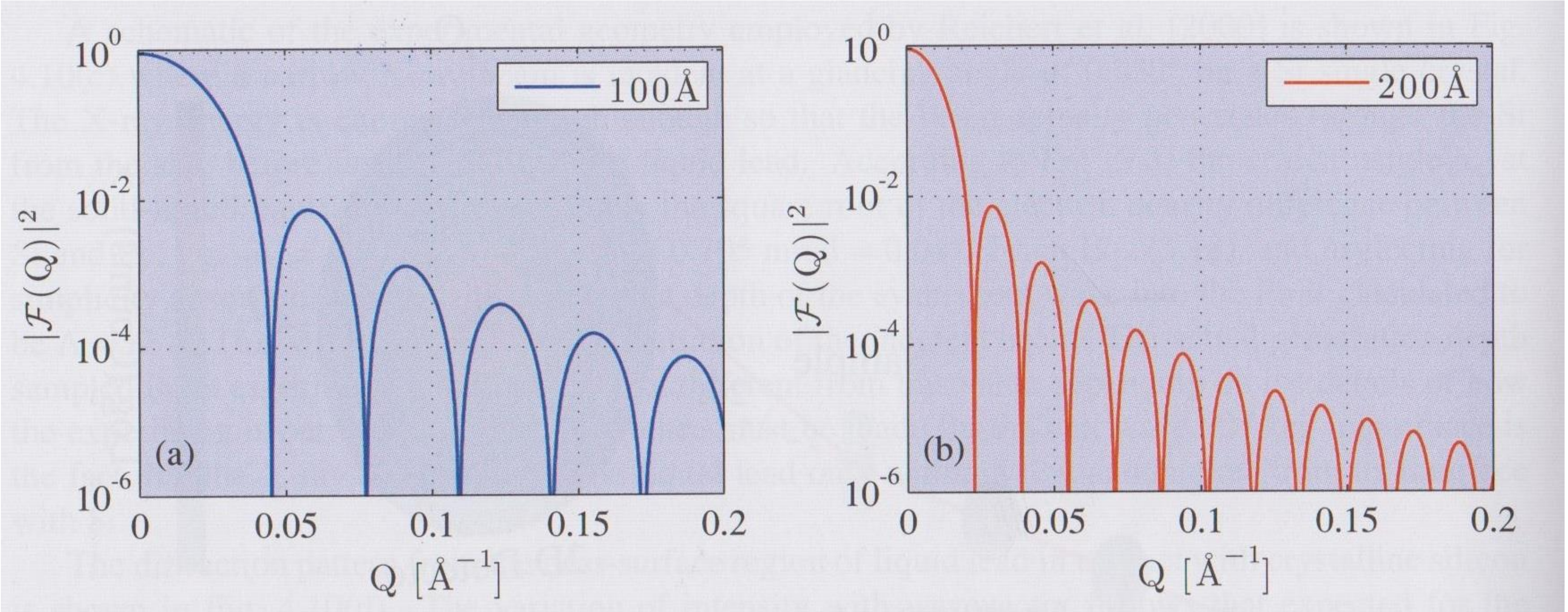
$Q \approx \xi = 2\pi / d_{Particle} = 2\pi / 628Å = 0.01\ Å^{-1}$

$\theta = \sin^{-1}(Q \bullet \lambda / 4\pi) = \sin^{-1}(0.01Å^{-1} \bullet 1Å / 4\pi) \approx 0.0456\ deg$

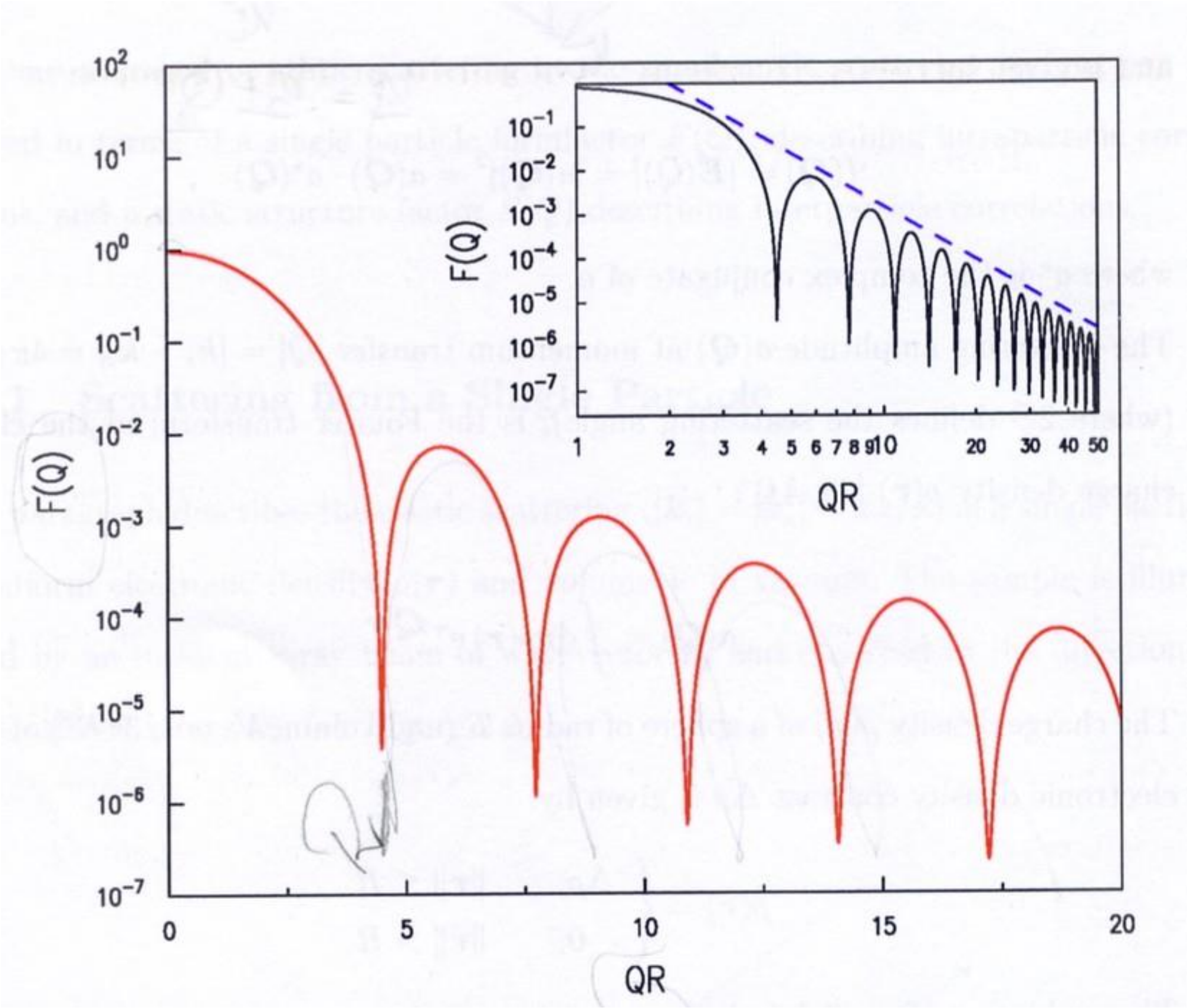
$d = L \bullet \tan(2\theta) = 2\ m \bullet 1.58 * 10^{-3} = 3.183\ mm$

Form Factor for Monodisperse Spheres

Monodisperse spheres of radius 10nm and 20 nm



Form Factor for Monodisperse Spheres



The Small Q Limit: Guinier Regime

For $QR \to 0$:

$$F(Q) \approx \frac{3}{(QR)^3}\left[QR - \frac{(QR)^3}{6} + \frac{(QR)^5}{120} = \cdots - QR\left(1 - \frac{(QR)^2}{2} + \frac{(QR)4}{24}\right)\right]$$

$$\approx 1 - \frac{(QR)^2}{10}$$

Thus:

$$I_{SAXS}(Q) \approx \Delta\rho^2\, V^2{}_p \left[1 - \frac{(QR)^2}{10}\right]^2 \approx \Delta\rho^2\, V^2{}_p \left[1 - \frac{(QR)^2}{5}\right]$$

Thus the QR → 0 limit can be used to determine the particle radius R via:

$$I_{SAXS}(Q) \approx \Delta\rho 2\, V^2{}_p \;\; e^{-\frac{(QR)^2}{5}} \qquad QR << 1\, [e^{-x} = 1 - x]$$

Thus: plotting ln $[I_{SAXS}(Q)]$ vs. Q^2 reveals a slope ~ $R^2/5$ ⇒ R

The Large Q Limit: Porod Regime

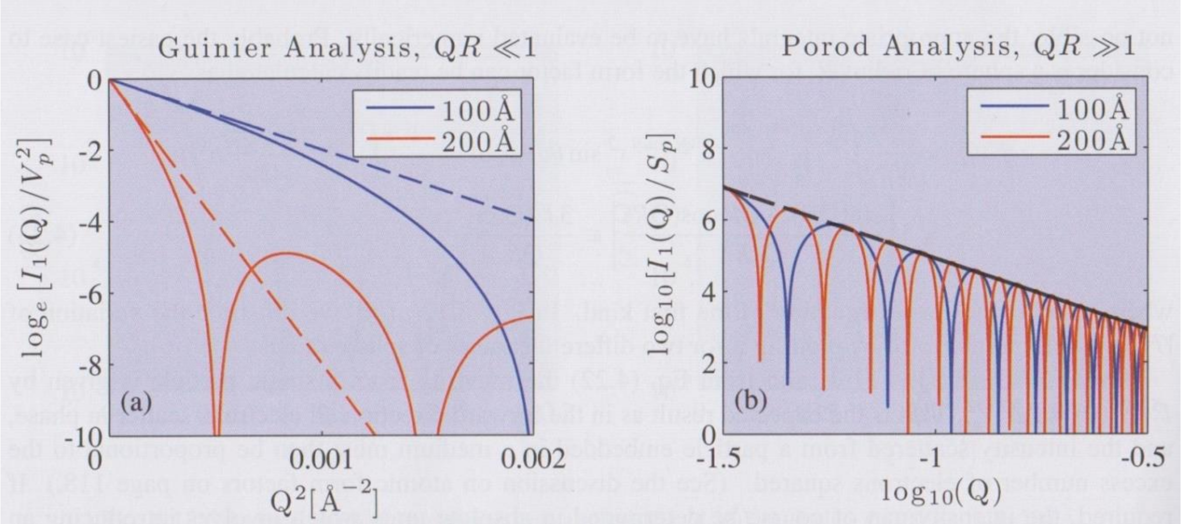
For QR >> 1: wavelength small compared to particle size

$$F(Q) = 3\left[\frac{\sin(QR)}{(QR)^3} - \frac{\cos(QR)}{(QR)^2}\right] \approx 3\left[-\frac{\cos(QR)}{(QR)^2}\right]$$

When QR >> 1 $\cos^2(x)$ oscillates towards ½ and

$$I_{SAXS}(Q) = 9\Delta\rho^2 V^2{}_p \frac{<\cos^2(QR)>}{(QR)4} = \frac{9\Delta\rho^2 V_p^2}{2(QR)^4}$$

Thus: $I_{SAXS}(Q) \sim \frac{1}{Q^4}$



Radius of Gyration

Radius of gyration: root mean sqare distance from the particle’s center

$$R_G = \frac{1}{V_p} \int_{vp} r^2 dV_p$$

$$R_G^2 = \frac{\int_{v_p} dV_p\, \rho_{sl,p}(r) r^2 dV_p}{\int_{v_p} \rho_{sI,p}(r) dV_p}$$

For uniform spheres: $R^2{}_G = \frac{3}{5} R^2$

$$I^{SAXS}(Q) \approx \Delta\rho^2\, V_P^2\, e^{(-(QR_G)^2/3}$$

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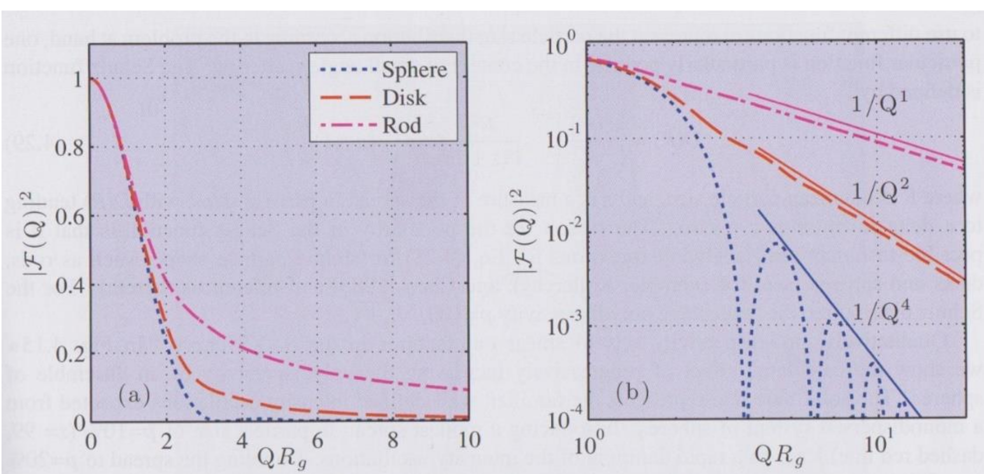
Form Factor and Particle Shape

$$F(Q) = \frac{1}{V_p} \int_{V_p} e^{iQr} dV_p$$

	$\lvert F(Q) \rvert^2$	R_G	Porod Exp.
Sphere (d=3)	$\left(\frac{3J_1(QR)}{QR}\right)^2$	$\sqrt{\frac{3}{5}}$ R	-4
Disc (d=3)	$\frac{2}{(QR)^2}\left(1 - \frac{J_1(2QR)}{QR}\right)$	$\sqrt{\frac{1}{2}}$ R	-2
Rod (d=1)	$\frac{2Si(QL)}{QL} - \frac{4\sin^2(QR/2)}{(QL)^2}$	$\sqrt{\frac{1}{12}}$ L	-1



with: $Si(x) \; {}_0\int^x \; \sin t/t \; dt$

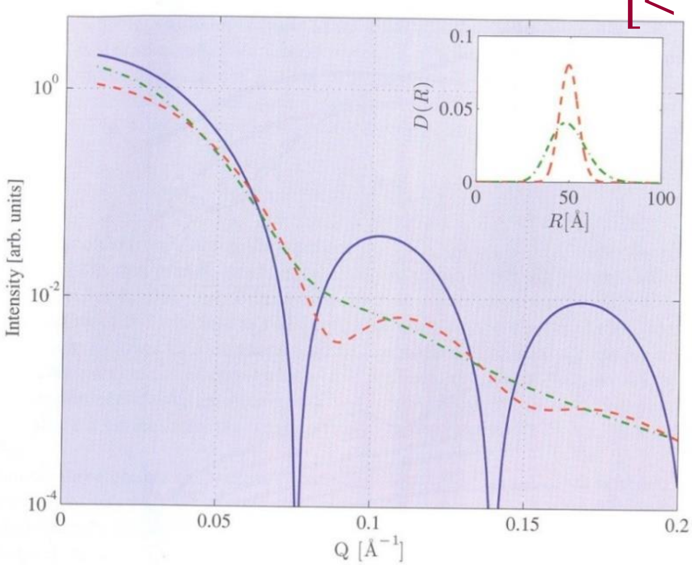
Polydispersity

Realistic ensembles of particles display a certain distribution of particle sizes that shall be disribed by a distribution function D(R). Thus the scattering intensity may be written as

$$I_{SAXS}(Q) = \Delta\rho 2\ 0\int\infty\ D(R)\ V^2{}_p\ |F(Q,R)|2\ dR$$

with $_0\int^\infty D(R)\, dR = 1$. A frequently used distribution function is the so-called Schultz function, where z is a measure of the polydispersity:

$$D(R) = \left[\frac{z+1}{<R>}\right]^{z+1} \frac{R^z}{\Gamma(z+1)}\, e^{\left(-(z+1)\frac{R}{<R>}\right)}$$



Structure Factor

Interparticle interactions:

S(Q): structure factor

Hard sphere structure factor:

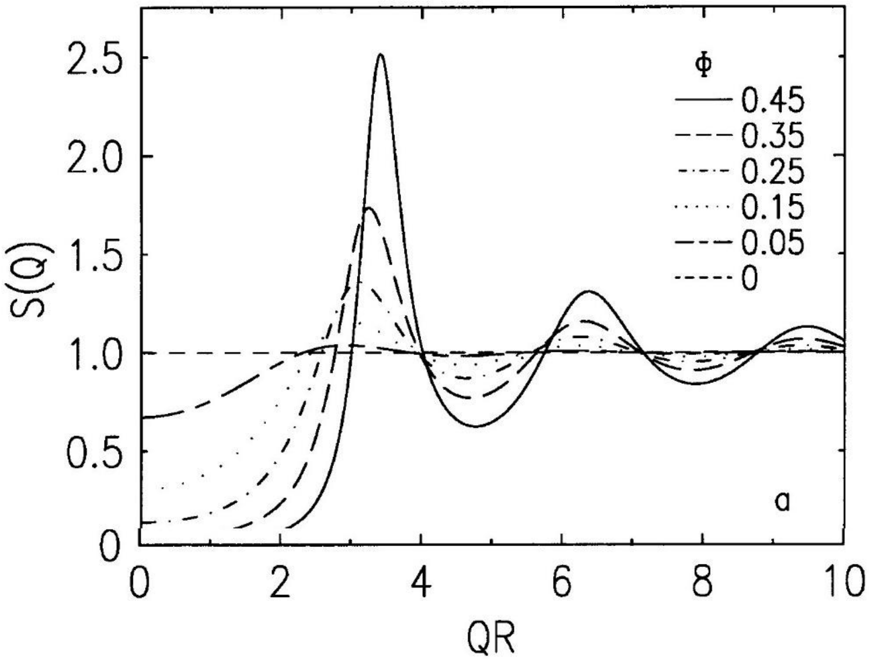
$V(r) = 0 \quad \text{for } r \geq d$

$V(r) = \infty \quad \text{for } r < d$

$$I_{SAXS}(Q) = \Delta\rho 2\, V^2{}_p\, |F(Q)|^2\, S(Q)$$

$$S(Q) = \frac{1}{nN} < \sum^N{}_{i,j}\; e^{i\mathbf{Q}(R_i - R_j)} >$$

$$= \int d^3r\, e^{iQr} \bullet g(r)$$



SAXS Experiment

- measure I(Q)
- model F(Q)
- for spherical particles I(Q)=F(Q)•S(Q)
- get and model S(Q)