Methoden moderner Röntgenphysik II

Streuung und Abbildung

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DESY
03.06.2014

HELMHOLTZ
ASSOCIATION

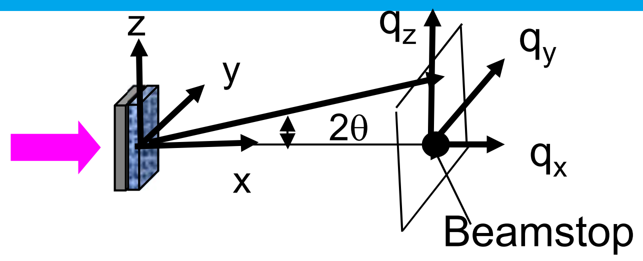
DESY

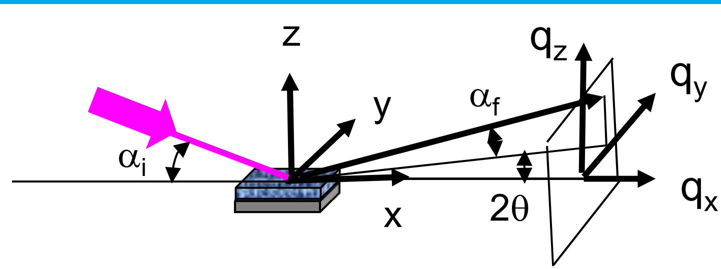
- Methoden moderner Röntgenphysik II:
  Streuung und Abbildung
- Vorlesung zum Haupt/Masterstudiengang Physik
  SS 2014 (Nr. 66-362)
- G. Grübel, M. Martins, E. Weckert
- Location:
  Hörs AP, Physik, Jungiusstrasse
  Tuesdays 12.45 – 14.15
  Thursdays 8:30 – 10.00
- Übungen: 2 SWS: Dienstag 14:30 – 16:00 (wenn vereinbart)
  (Nr. 66-363)
  SemRm 4
- **EXKURSION: 1.7.2014, ab 14:15? Bestätigung!!!**

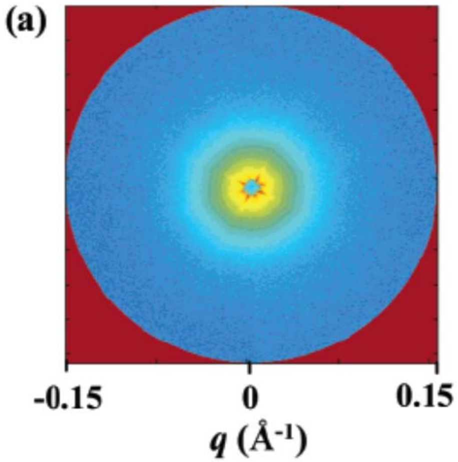
Outline I

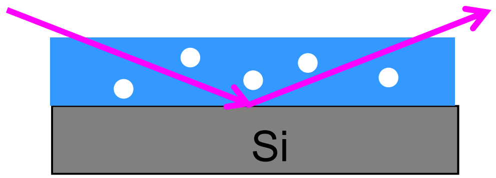
- 03.06 : Small-Angle X-ray Scattering (SAXS)
- 05.06 : Applications &
  A short excursion into Polymeric materials
- 17.06 : Grazing incidence SAXS (GISAXS)
- 19.06 : In-situ studies of metal layer growth (M. Schartzkopf)
- 24.06 : The polymer-metal interface – application of GISAXS
  On the route to organic electronics

T-SAXS vs. GISAXS

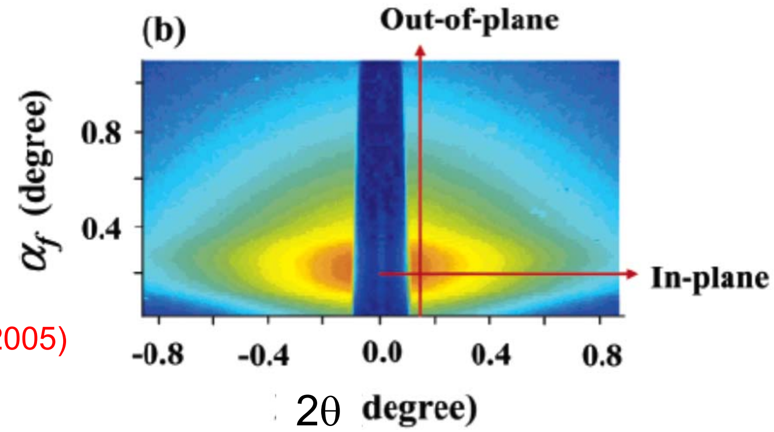








Lee et al., Macromolecules, 38, 8991 (2005)



- Easy measurement
- Easy analysis
- In-plane information (q_y,q_z)
- Any possible scattering from substrate
- Transparency of substrate
- High energy

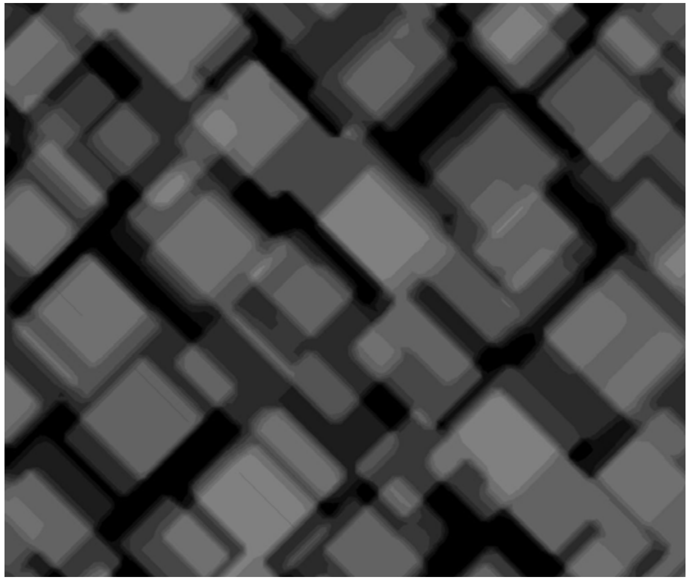
- Strong intensity
- Easy preparation of samples
- Full information (q_x,q_y,q_z)
- Scattering from surface / internal structure
- Scattering from reflected AND transmitted beam
- Refraction effects (DWBA)
- Special setup

Aim

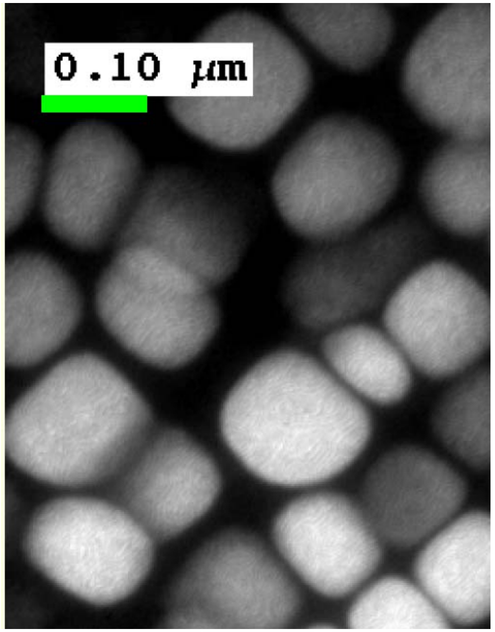
> To understand the **structure – property relation** of **materials** on **multiple length scales**

- **q-resolution**
- Maximum q-value
- **Beam size**

- Real pieces & materials
- Model systems
- Nanotechnology



Courtesy: R. Gilles (TUM)



http://news.thomasnet.com/companystory/GE-Gas-Turbine-Technology-Selected-for-Pearl-GTL-Project-in-Qatar-495497

Outline II - today

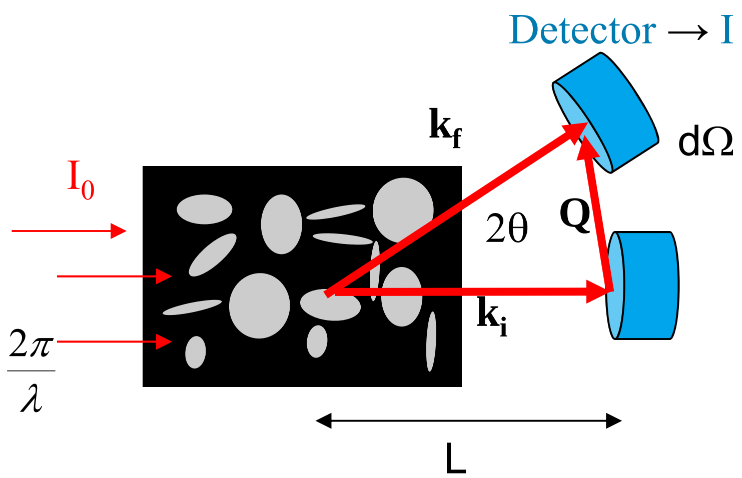
- ➡ SAXS – Introduction

Neutrons, X-rays and Light: Scattering Methods Applied to Soft Condensed Matter.
Eds: P. Lindner, Th. Zemb. North Holland Delta Series, Elsevier, Amsterdam (2002)
ISBN: 0-444-51122-9

- Instrumentation
  - P03/MiNaXS @ PETRA III
- Bulk materials ➔ Transmission U/SAXS:
  - Porous materials
  - Ni-base superalloys
  - Droplet drying

Cross-section

> Differential cross section



$$d\sigma = \frac{I}{I_0}(L^2 d\Omega)$$

$$\frac{d\sigma}{d\Omega} = \frac{I}{I_0}(L^2) \quad \Rightarrow \frac{d\Sigma}{d\Omega} = \frac{1}{V}\frac{d\sigma}{d\Omega}$$

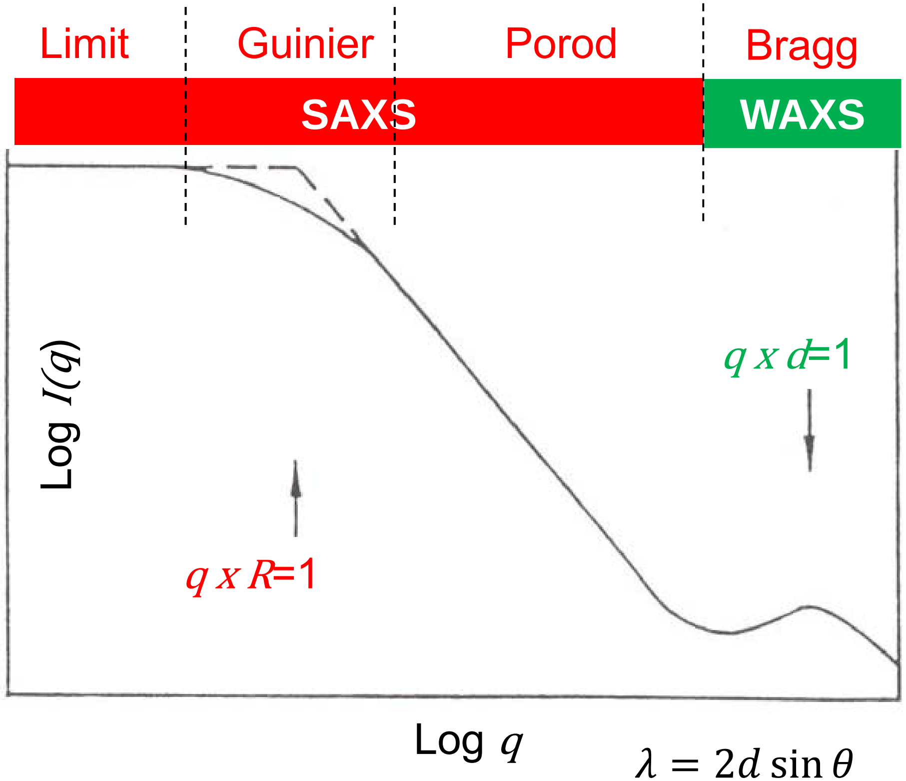
V=Sample volume

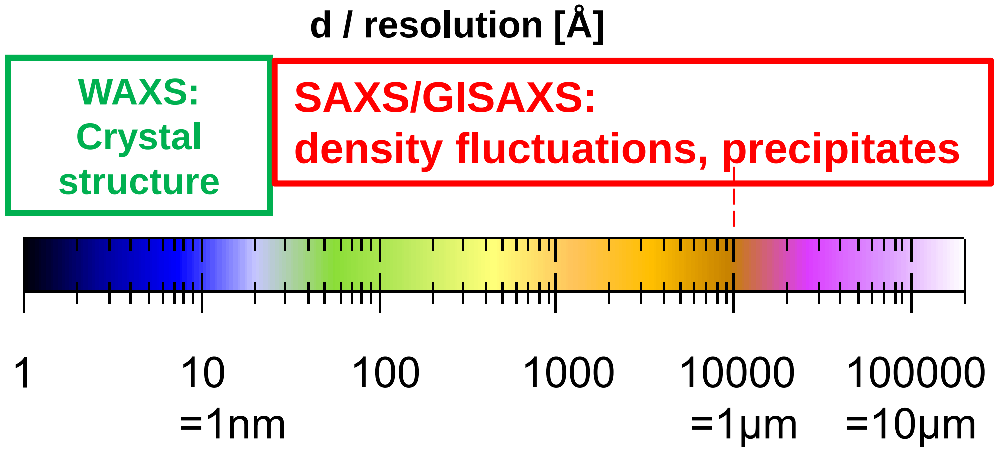
$$\vec{q} = \overrightarrow{k_f} - \overrightarrow{k_i} \qquad |\vec{k}_f| = |\vec{k}_i| = \frac{2\pi}{\lambda} \qquad |\vec{q}| = 2\frac{2\pi}{\lambda}\sin(\theta)$$

> Scattering occurs due to density differences

WAXS, SAXS, GISAXS…

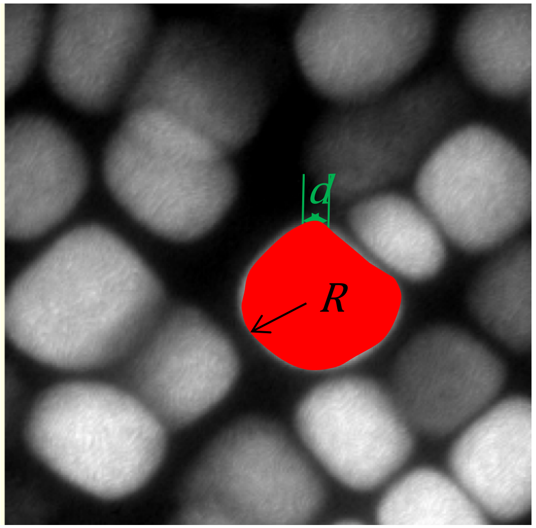
Source: Streumethoden zur Untersuchung kondensierter Materie
1996; ISBN 978-3-89336-180-9





$$\lambda = 2d \sin\theta$$

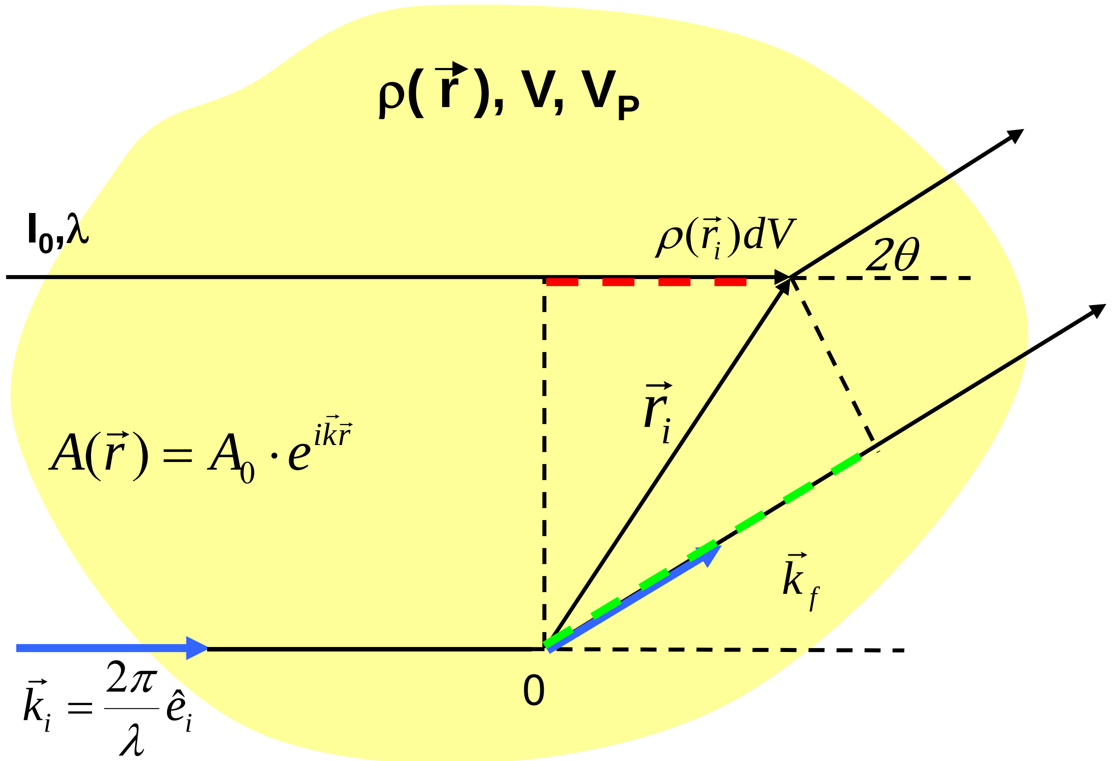
$$\lambda = 1.54\text{Å}$$

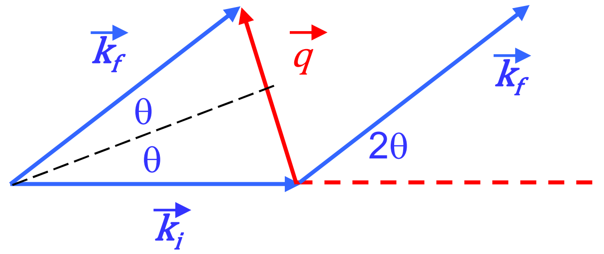


- R~particles "radius"
- d~interatomic distance
- SAXS: $\theta < 5°$

Scattering amplitude

- Interference in far field

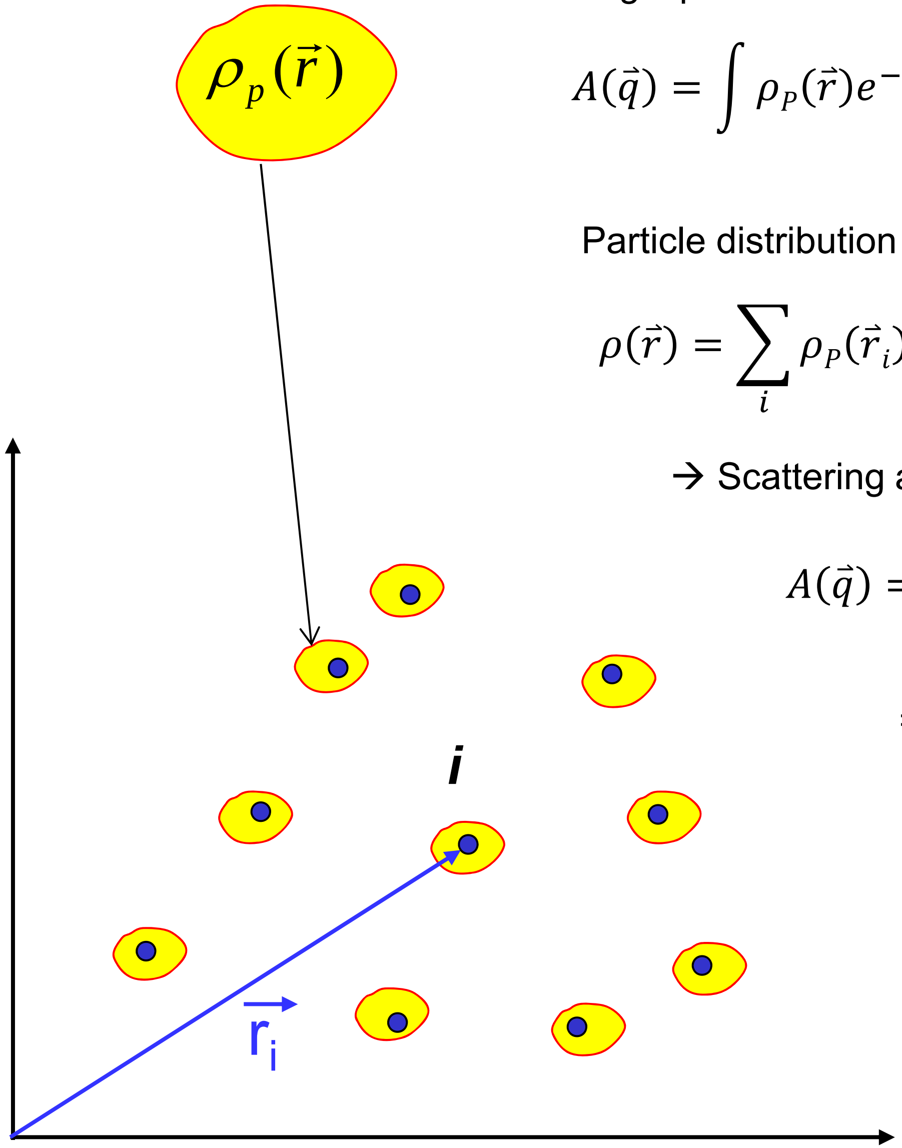




$$\left|\vec{q}\right| = \frac{4\pi}{\lambda}\sin\theta$$

- Phase difference: $\Delta\varphi_i = (\vec{k}_f - \vec{k}_i)\cdot\vec{r}_i = \vec{q}\cdot\vec{r}_i$
- Scattering amplitude: $A(\vec{q}) = \int \rho(\vec{r})e^{-i\vec{q}\vec{r}}dV = \int \rho(\vec{r})e^{-i\vec{q}\vec{r}}d^3\vec{r}$
- Intensity: $I\left(\vec{q}\right) = \frac{1}{V}\left|A\left(\vec{q}\right)\right|^2$

Form factor and structure factor: Fourier transform



Single particle: Fourier transformation

$$A(\vec{q}) = \int \rho_P(\vec{r})e^{-i\vec{q}\vec{r}}dV = \int \rho_P(\vec{r})e^{-i\vec{q}\vec{r}}d^3\vec{r}$$

Particle distribution function G(**r**) → Electron density distribution

$$\rho(\vec{r}) = \sum_i \rho_P(\vec{r}_i) = \int \rho_P(\vec{r}')G(\vec{r}-\vec{r}')d^3r' = \rho_P(\vec{r}) * G(\vec{r})$$

→ Scattering amplitudes of the whole arrangement

$$A(\vec{q}) = \int \rho(\vec{r})e^{-i\vec{q}\vec{r}}dV = \int [\rho_P(\vec{r}) * G(\vec{r})\,]e^{-i\vec{q}\vec{r}}d^3\vec{r}$$

$$= \int \rho_P(\vec{r})e^{-i\vec{q}\vec{r}}dV \cdot \int G(\vec{r})e^{-i\vec{q}\vec{r}}dV$$

→ Scattered Intensity

$$I(\vec{q}) = \frac{1}{V}|A(\vec{q})|^2 = P(\vec{q})S(\vec{q})$$

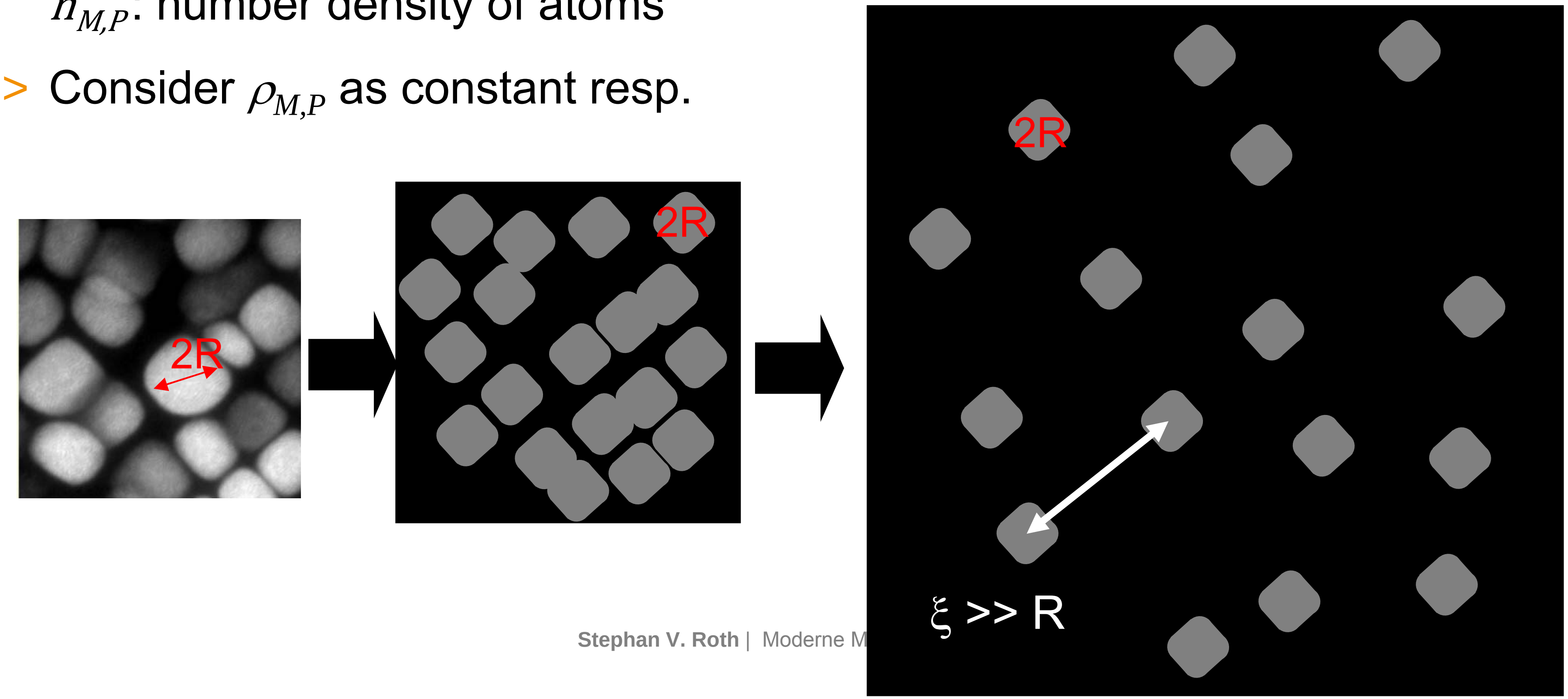
Form factor Structure factor

Two-phase model: Dilute systems

- Only form of particle relevant
- Matrix M, volume fraction Φ
  Particles P, volume fraction $(1-\Phi)$
  Electron density: $\rho_{M,P}=n_{M,P}*f_{M,P}$

  $f_{M,P}$: atomic form factor („extension of the electron cloud“, resonances)
  $n_{M,P}$: number density of atoms
- Consider $\rho_{M,P}$ as constant resp.

ASAXS



Two phase Model

> Scattering amplitude:

$$A(\vec{q}) = \int \rho(\vec{r}) e^{-i\vec{q}\vec{r}} d^3\vec{r} = \int_{\Phi V} \rho_M(\vec{r}) e^{-i\vec{q}\vec{r}} d^3\vec{r} + \int_{(1-\Phi)V} \rho_P(\vec{r}) e^{-i\vec{q}\vec{r}} d^3\vec{r}$$

$$A(\vec{q}) = (\rho_M - \rho_P) \int_{\Phi V} e^{-i\vec{q}\vec{r}} d^3\vec{r}$$

$$A(\vec{q}) = \Delta\rho \int_{\Phi V} e^{-i\vec{q}\vec{r}} d^3\vec{r}$$

> $I(\vec{q}) = \frac{1}{V} |A(\vec{q})|^2 \sim \Delta\rho^2$

> Porod Invariant Q (Porod, 1982):
$\mathrm{Q} = \int I(\vec{q}) d^3\vec{q} = 4\pi \Phi(1-\Phi)\Delta\rho^2$

Ableiten!
Mittelung <..> erklären S.25, S.51

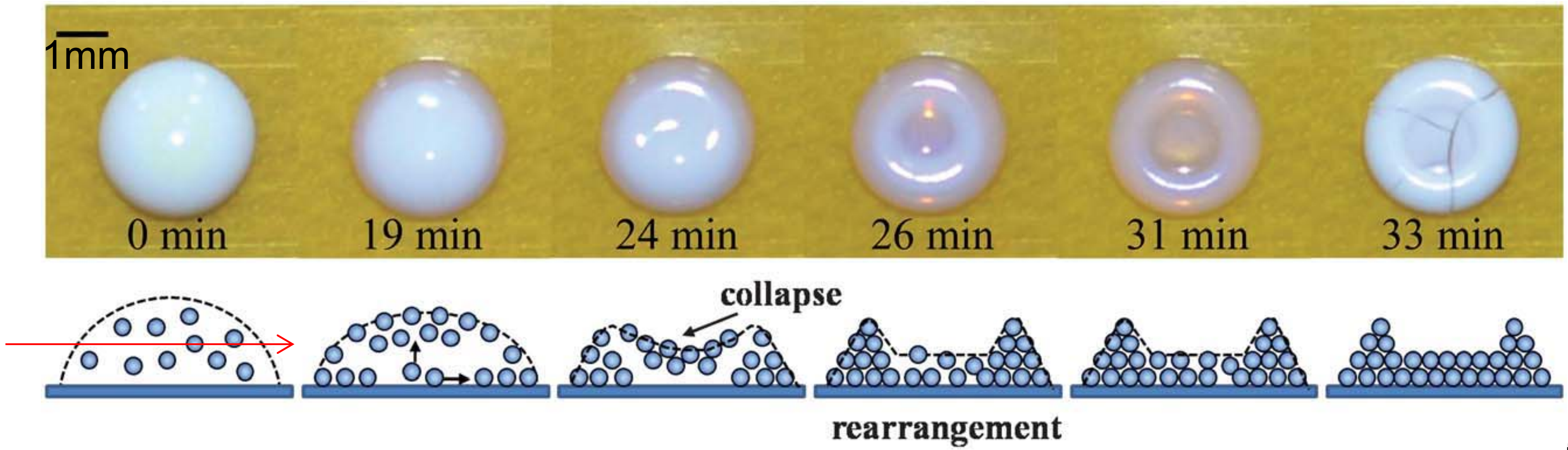
> Only dependent on density contrast $\Delta\rho$

Herleitung Porod-Invariante

> Siehe Handzettel und Übung

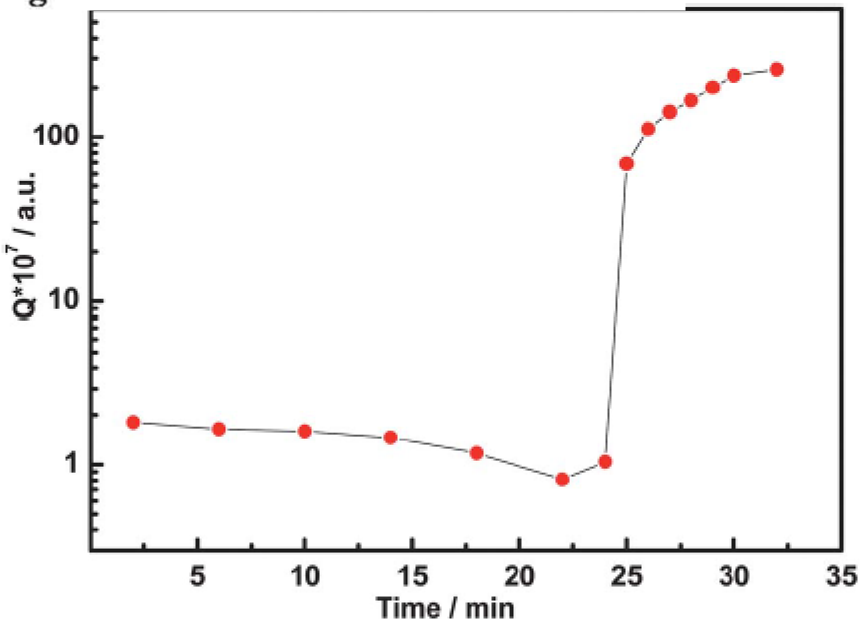
Porod Invariant - practical application

> Colloidal solution: drying thick droplet



> Evaporation of water:

- Irradiated volume becomes smaller: shrinking
- Distance of colloidal partices decreases, $\Phi \rightarrow 1$
- $\Delta\rho$ increases (air!), as water removed from interstitial sites



Chen et al., Soft Matter 8, 12093 (2012)