NEUTRON GRATING INTERFEROMETRY
PART II

QUANTITATIVE DFI

Alexander Backs
alexander.backs@frm2.tum.de
nGI reveals scattering

- from small structures (~ μm)
- under very small angles

What does that mean exactly?
Quantitative DFI: Size Matters

Polysterene Colloids in Solution

- varying particle diameter
- constant volume fraction

- constant absorption
- varying DFI value

Model Case: One Single Scattering Angle

without sample:

\[ V_{ob} = \cos(x) \]
Origin of the DFI

Model Case: One Single Scattering Angle

without sample:

$$V_{ob} = \cos(x)$$

with sample:

$$V_s = \frac{1}{2} \cos(x + \theta) + \frac{1}{2} \cos(x - \theta)$$
Origin of the DFI

Model Case: One Single Scattering Angle

without sample:

\[ V_{ob} = \cos(x) \]

with sample:

\[ V_s = \frac{1}{2} \cos(x + \vartheta) + \frac{1}{2} \cos(x - \vartheta) \]
\[ V_s = \cos(x) \cos(\xi_{G1} q_x) \]

\[ \vartheta = \xi_{G1} q_x \]
\[ \xi_{G1} = \lambda \frac{L_s, eff}{p_2} \]

\[ DFI = \frac{V_s}{V_{ob}} = \cos(\xi_{G1} q_x) \]
Origin of the DFI

Real Case: Distribution of Scattering Angles

\[ DFI = \cos(\xi_{GI} q_x) \]

\[ DFI = \int S(q_x) \cos(\xi_{GI} q_x) \, dq_x \]
Origin of the DFI

Real Case: Distribution of Scattering Angles

DFI = \cos(\xi_{G1} q_x)

\[ DFI = \int S(q_x) \cos(\xi_{G1} q_x) \, dq_x \]

What defines \( S(q_x) \)?

\( S(q_x) \)

"probability of scattering a neutron with a certain momentum transfer \( q_x \)"
Reciprocal Space: the differential scattering cross section (looking at momentun)

\[ d\sigma(q) = \frac{\text{neutrons scattered into } d\Omega}{\text{incoming neutrons per unit area}} \]
\[ S(q_x) : A \text{ Bit of Scattering Theory} \]

**Reciprocal Space:** the differential scattering cross section (looking at momentum)

\[ d\sigma(q) \frac{d\Omega}{d\Omega} = \frac{\text{neutrons scattered into } d\Omega}{\text{incoming neutrons per unit area}} \]

**Real space:** the pair correlation function (looking at space coordinates)

\[ \gamma(r) = \int_v \Delta \rho(R) \Delta \rho(R + r) dR \]

Distribution of scattering strength
S(q_x) : A Bit of Scattering Theory

**Reciprocal Space:** the differential scattering cross section (looking at momentun)

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Distribution of scattering strength
Step 1: no scattering along the beam direction \( q_z = 0 \)

\[
\frac{d\sigma(q)}{d\Omega} \rightarrow \frac{d\sigma(q_x, q_y, 0)}{d\Omega}
\]

\[
G(x, y) = \int \gamma(x, y, z) \, dz
\]
S(q_x) : Reducing the Dimensions

**Step 1:** no scattering along the beam direction \( q_z = 0 \)

\[
\frac{d\sigma(q)}{d\Omega} \rightarrow \frac{d\sigma(q_x, q_y, 0)}{d\Omega}
\]

\[G(x, y) = \int \gamma(x, y, z) \, dz\]

**Step 2:** projection along the grating lines \( q_y = -\infty \rightarrow +\infty \)

\[
\left( \frac{d\sigma(q_x)}{d\Omega} \right)_{\text{slit}} = \int \frac{d\sigma(q_x, q_y, 0)}{d\Omega} \, dq_y
\]

\[G(x, y) \rightarrow G(x, 0)\]
Quantitative DFI: The Formula

Reciprocal Space:

\[ S(q_x) \approx \left( \frac{d\sigma(q_x)}{d\Omega} \right)_{slit} \]

\[ q_z = 0 \]
\[ q_y = -\infty \rightarrow +\infty \]

\[ DFI = \int S(q_x) \cos(\xi_{Gl} q_x) \, dq_x \]

Quantitative DFI: The Formula

Reciprocal Space:

\[ S(q_x) \approx \left( \frac{d\sigma(q_x)}{d\Omega} \right)_{\text{slit}} \]

\[ q_z = 0 \]
\[ q_y = -\infty \rightarrow +\infty \]

\[ DFI = \int S(q_x) \cos(\xi_{GI} q_x) \, dq_x \]

Real Space:

\[ DFI = \exp \left[ \Sigma t \left( \frac{G(\xi_{GI})}{G(0)} - 1 \right) \right] \]

Total scattering crosssection \[ \Sigma = (\Delta \rho)^2 \lambda^2 \Phi_v \frac{G(0)}{\gamma(0)} \]

sample thickness \[ t \]

nGI correlation length \[ \xi_{GI} \]
A Simple Example: Hard Spheres

Polystyrene Colloids in Solution

Pair Correlation Function
A Simple Example: Hard Spheres

Polystyrene Colloids in Solution

Pair Correlation Function

**calculate:**

\[ \gamma(x, y, z) \]
\[ G(x, y) \]
\[ G(x, 0) \]

**fourier transform:**

\[ \frac{d\sigma(q_x, q_y, q_z)}{d\Omega} \]
\[ \frac{d\sigma(q_x, q_y, 0)}{d\Omega} \]
\[ \left( \frac{d\sigma(q_x)}{d\Omega} \right)_{slit} \]

Real Space
Reciprocal Space
Polysterene Colloids in Water

Real Space: Pair Correlation function

Reciprocal Space: Scattering cross section

Polysterene Colloids in Water

\[ DFI = \exp \left( \Sigma t \left( \frac{G(\xi_{GI})}{G(0)} - 1 \right) \right) \]

**R dependence:**
- \( G = G(R) \)
- \( \Sigma = \Sigma(R) \)

**λ dependence:**
- \( \xi_{GI} = \xi_{GI}(\lambda) \)
- \( \Sigma = \Sigma(\lambda) \)

DFI depends only on one value of the pair correlation function $G(\xi_{GI})$.

More information can be gained by:

- Changing $G$
- Different particle sizes
- Only possible in rare cases
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- Changing $\xi_{GI}$
  - Change the setup or Sample position
  - Various geometric constraints
  - Tedious callibrations
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More information can be gained by:

- **Changing $G$**
  - Different particle sizes
  - Only possible in rare cases

- **Changing $\xi_{GI}$**
  - Change the setup or Sample position
  - Various geometric constraints
  - Tedious callibrations
  - Only a small range is accessible

- **Vary the wavelength**
Inhomogeneous Scattering

\[ \frac{d\sigma}{d\Omega} \]

\[ \int dq_y \]

Homogenous

\[ \frac{d\sigma}{d\Omega} \]

\[ \int dq_y \]

Inhomogenous

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Inhomogeneous Scattering

\[
\int dq_y \left( \frac{d\sigma(q_x)}{d\Omega} \right)_{slit}
\]

depends on the relative orientation of sample and gratings.
Inhomogeneous Scattering

\[
\frac{d\sigma(q_x)}{d\Omega} \quad \text{depends on the relative orientation of sample and gratings}
\]

\[
DFI(\omega) = \exp \left[ \Sigma t \left( \frac{G(\xi_{GI} \cos(\omega), -\xi_{GI} \sin(\omega))}{G(0)} - 1 \right) \right]
\]
Anisotropic scattering in Brass

Extrusion Moulded Brass: anisotropic
• production
• crystallites
• scattering

Anisotropic scattering in Brass

Different distribution of crystallite size in x and y direction

- Bi gaussian scattering cross section

\[ DFI(\omega) = \exp \left[ -\frac{\xi GI}{2} \left( \sigma_x^2 + \left( \sigma_y^2 - \sigma_x^2 \right) \sin^2(\omega - \varphi) \right) \right] \]

\[ \sigma_{an} = \sigma_x^2 - \sigma_y^2 \]

\( \sigma_x^2 \)

\( \sigma_y^2 \)

Anisotropic scattering in Brass

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DFI(\omega) = \exp \left[ -\frac{\xi_{GI}}{2} (\sigma_x^2 + (\sigma_y^2 - \sigma_x^2)\sin^2(\omega - \varphi)) \right] \\
\sigma_{an} = \sigma_x^2 - \sigma_y^2
\]

Magnetic Domains in Superconductors

Normal Conductor

\[ \overrightarrow{B} \]

Superconductor

\[ \overrightarrow{B} \]

low field

Meissner state

high field

Schubnikov state
Magnetic Domains in Superconductors

Normal Conductor

\[ \vec{B} \]

Superconductor

\[ \vec{B} \]

low field

\[ \vec{B} \]

high field

intermediate mixed state

bubble structure

laminar structure

\[ \vec{B} \]


The Intermediate Mixed State in Niobium

Field Cooling into the IMS

What changes?
• domain size
• domain density
• scattering contrast
The Intermediate Mixed State in Niobium

Suppression of the IMS

- Additional field enters the sample
  - IMS in the center
  - FLL at the edge
  - pinning along crystal axes

Heterogeneous Phase transition

From USANS to nGI

\[
\left( \frac{d\sigma(q_x)}{d\Omega} \right)_{\text{slit}}
\]

\[
G(x, 0)
\]

\[
DFI = \exp \left[ \Sigma t \left( \frac{G(\xi_{GI})}{G(0)} - 1 \right) \right]
\]

From USANS to nGI

Magnetic Field Scan

Domain size changes
(USANS result)

Wavelength Scan

Probed $\xi_{GI}$ changes