Jülich Centre for Neutron Science

FRM II
Forschungs-Neutronenquelle
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MLZ
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Interference functions

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MLZ is a cooperation between:

JÜLICH
FORSCHUNGSZENTRUM

Helmholtz-Zentrum
Geesthacht
Zentrum für Material- und Küstenforschung

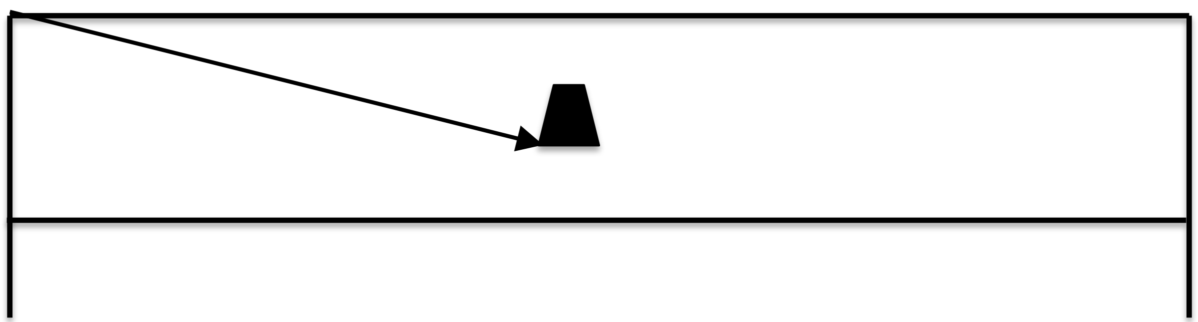
Technische Universität München

Overview

- The differential cross section
- Statistical expectation values
  - Decoupling approximation
  - Local Monodisperse approximation
  - Size-position coupling
- Completely disordered particles
- One-dimensional lattice
- Two-dimensional lattice
- Radial paracrystal
- Two-dimension paracrystal
- GUI with a scent of Python

Particle shapes and positions

- Particles defined by shapes and positions



Scattering cross section

- Scattering amplitude: $\left\langle \Psi_i \middle| \delta v \middle| \Psi_f \right\rangle = \sum_i \int d^3r \, e^{iq_{//}\cdot r_{//}} \sum_{k=1}^{4} A_k e^{iq_{kz}z} S_i(r - R_i)$

$$= \sum_i e^{iq_{//}\cdot R_{i//}} \int d^3r \, e^{iq_{//}\cdot r_{//}} \sum_{k=1}^{4} A_k e^{iq_{kz}z} S_i(x, y, z - R_{iz})$$

$$= \sum_i e^{iq_{//}\cdot R_{i//}} F_i^{DWBA}(q)$$

- Differential cross section

$$\frac{1}{N}\frac{d\sigma}{d\Omega} = \frac{1}{N}\left|\left\langle \Psi_i \middle| \delta v \middle| \Psi_f \right\rangle\right|^2$$

$$= \frac{1}{N}\sum_i \left|F_i^{DWBA}(q)\right|^2 + \frac{1}{N}\sum_{i \neq j} e^{iq_{//}(R_{i//}-R_{j//})} F_i^{DWBA}(q) \bar{F}_j^{DWBA}(q)$$

Statistical average

- Integrate over probability density function:

$$\langle \cdots \rangle \equiv \int \prod_i dR_i d\alpha_i P(\{\alpha_i\},\{R_i\}) \cdots$$

- Apply chain rule:

$$P(\{\alpha_i\},\{R_i\}) = P(\{R_i\} \big| \{\alpha_i\}) \cdot P(\{\alpha_i\})$$

Decoupling approximation

- Probability density: $P(\{R_i\}|\{\alpha_i\}) = P(\{R_i\})$

$$\frac{1}{N}\frac{d\sigma}{d\Omega} = \left\langle \left| F_\alpha^{DWBA} \right|^2 \right\rangle_\alpha - \left| \left\langle F_\alpha^{DWBA} \right\rangle_\alpha \right|^2$$

$$+ \sum_{i \neq j} \int d\alpha_i \, d\alpha_j P(\alpha_i, \alpha_j) F_{\alpha_i}^{DWBA} \overline{F}_{\alpha_j}^{DWBA} S$$

$$= I_d + I_c$$

- Interference function: $S = 1 + \rho_S^{-1} \int d^2 R \, e^{iq_{//} \cdot R} P(R)$

- For single particle type:

$$\frac{1}{N}\frac{d\sigma}{d\Omega} = I_c$$

Local monodisperse approximation

- Probability density: $P(R_i - R_j | \alpha_i, \alpha_j) = \delta(\alpha_i - \alpha_j) P(R_i - R_j | \alpha_i)$

$$\frac{1}{N}\frac{d\sigma}{d\Omega} = \int d\alpha_i P(\alpha_i) \left| F_{\alpha_i}^{DWBA} \right|^2 S_{\alpha_i}$$

- Meaning:
  - Different spatially separated domains
  - Mixed particles, but no correlation between different particle ensembles
  - Just an ad hoc approximation

Size-position coupling approximation

- Nearest neighbor separation depends on the ‘size’ of the two particle types involved
- Only implemented for radial paracrystal, where the mean separation is linearly dependent on the sizes of the particles

No interference

- No correlation between different positions: $P(R) = \rho_S^2$
- Only incoherent superposition over different particle types remains:

$$\frac{1}{N}\frac{d\sigma}{d\Omega} = \left\langle \left| F_\alpha^{DWBA} \right|^2 \right\rangle_\alpha$$

Lattices and paracrystals

- Python scripts showing correlation
- GUI demo