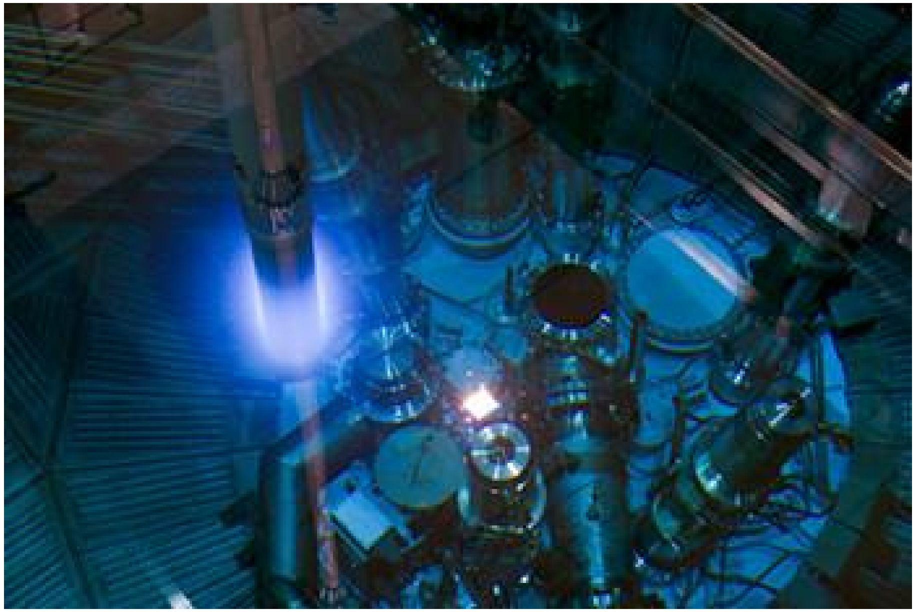
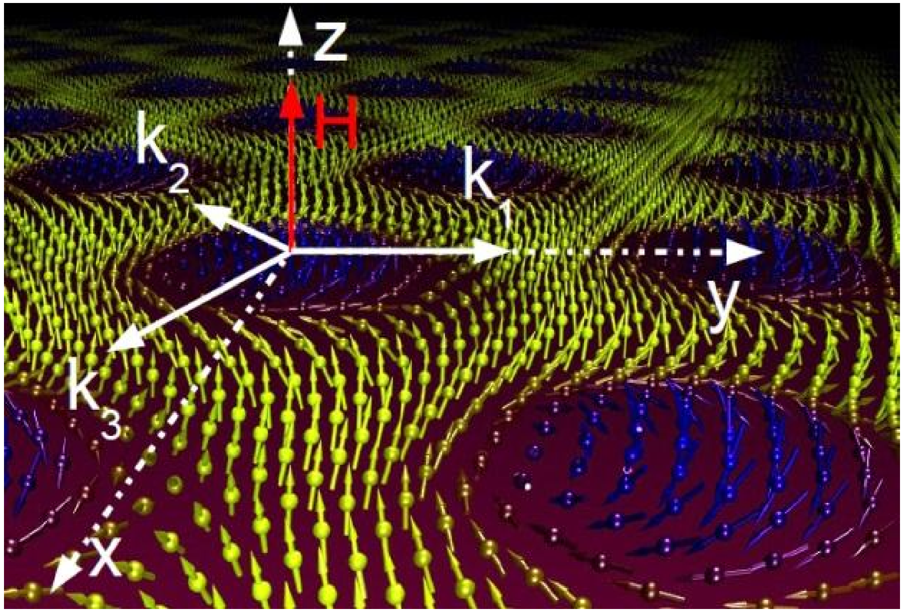
FRM II
Forschungs-Neutronenquelle
Heinz Maier-Leibnitz

MLZ
Heinz Maier-Leibnitz Zentrum

Physics with Neutrons I, WS 2015/2016





Lecture 6, 23.11.2015

MLZ is a cooperation between:

JÜLICH FORSCHUNGSZENTRUM

Helmholtz-Zentrum Geesthacht
Zentrum für Material- und Küstenforschung

TUM
Technische Universität München

Organization

Visit FRM II : 21.12.2015

10:15 – 13:00 (after the lecture)

Valid ID necessary!!!

Exam (after winter term)

- Registration: via TUM-Online between 16.11.2015 – 15.1.2015
- Email: sebastian.muehlbauer@frm2.tum.de for date arrangement
- 30min oral exam

3.3 Reminder: Coherent and incoherent scattering

Assume a large sample with statistically variations of b_j

No correlations among b: $\overline{b_{j'} b_j} = (\overline{b})^2, j' \neq j$

$$\overline{b_{j'} b_j} = (\overline{b^2}), j' = j$$

Double differential crosssection spilts up into two terms:

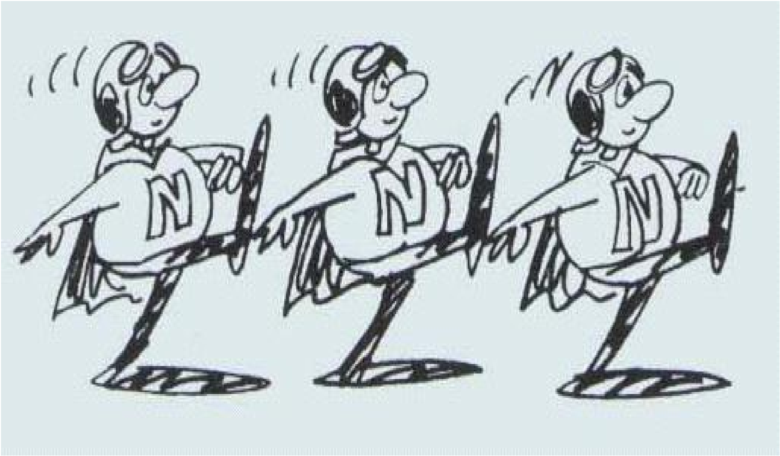
$$\left(\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega \mathrm{d}E'}\right)_{coherent} = \frac{\sigma_{coh.}}{4\pi} \frac{k'}{k} \frac{1}{2\pi\hbar} \sum_{j,j'} \int_{-\infty}^{\infty} \underline{\left\langle e^{i\kappa R_{j'}(0)} e^{-i\kappa R_j(t)} \right\rangle} e^{-i\omega t} \mathrm{d}t$$

$$\left(\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega \mathrm{d}E'}\right)_{incoherent} = \frac{\sigma_{inc.}}{4\pi} \frac{k'}{k} \frac{1}{2\pi\hbar} \sum_{j,j'} \int_{-\infty}^{\infty} \underline{\left\langle e^{i\kappa R_j(0)} e^{-i\kappa R_j(t)} \right\rangle} e^{-i\omega t} \mathrm{d}t$$

$$\sigma_{coh.} = 4\pi \overline{b}^2 \qquad \sigma_{inc.} = 4\pi (\overline{b^2} - \overline{b}^2)$$

3.3 Reminder: Coherent and incoherent scattering

Coherent



Spatial and temporal correlations between different atoms

- Interference effects:
- Given by average of b
  Bragg scattering

Incoherent

Spatial and temporal correlations between the same atom

- Constant in Q
- Given by variations in b due to spin, disorder, random atomic motion....

4.1 Elastic scattering from a single crystal: Static correlations only!

Starting point: Coherent elastic cross-section

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\mathrm{d}E'} = \frac{k'}{k}\frac{1}{2\pi\hbar}\sum_{j,j'} b_j b_{j'} \int_{-\infty}^{\infty} \left\langle e^{-i\kappa R_{j'}(0)} e^{-i\kappa R_j(t)} \right\rangle e^{-i\omega t}\mathrm{d}t$$

Sample: Single X-tal in thermal equilibrium, consider static correlations!

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \int_{\infty}^{\infty} \frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\mathrm{d}E'}\mathrm{d}(\hbar\omega) = \sum_{j,j'} b_j b_{j'} \left\langle e^{-i\kappa R_{j'}} e^{-i\kappa R_j} \right\rangle$$

Drop the operator formalism for R_j as we look at static correlations

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}_{coh.el} = \langle b\rangle^2 \sum_{j,j'} e^{-i\kappa(R_{j'}-R_j)}$$

➡ Information on the position of the atoms

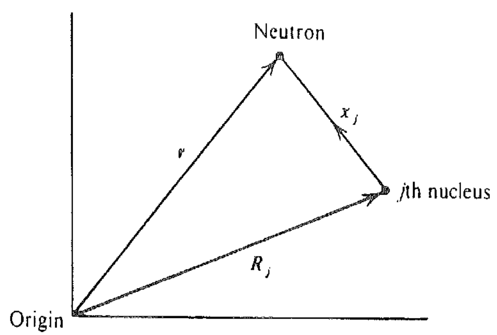
$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}_{inc.} = (\langle b^2\rangle - \langle b\rangle^2) \sum_{j=j'} e^{-i\kappa(R_{j'}-R_j} = N(\langle b^2\rangle - \langle b\rangle^2)$$

➡ Isotropic, constant background

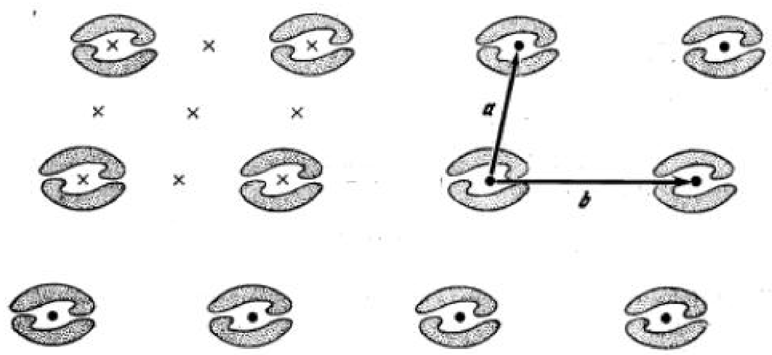
4.1 Elastic scattering from a single crystal: lattice sums

What we used:

Fig. 2.1 Coordinates of nucleus and neutron.



Our sample is a periodic crystal!



Crystal= Basis+lattice

$$\frac{d\sigma}{d\Omega}_{coh.el} = \langle b \rangle^2 N_0 \sum_T e^{i\vec{\kappa}\vec{T}} \quad \text{with} \quad \vec{R}_{j'} - \vec{R}_j = \vec{T}$$

Lattice sum: $$\sum_{\vec{l}} e^{i\vec{\kappa}\vec{l}} = \frac{(2\pi)^3}{v_0} \sum_{\vec{\tau}} \delta(\vec{\kappa} - \vec{\tau})$$

Real space lattice

Reciprocal space lattice

4.1 Elastic scattering from a single crystal: Braggs law

Lattice sum:

$$\sum_{\vec{l}} e^{i\vec{\kappa}\vec{l}} = \frac{(2\pi)^3}{v_0} \sum_{\vec{\tau}} \delta(\vec{\kappa} - \vec{\tau})$$

Real space lattice

Reciprocal space lattice

Braggs law:

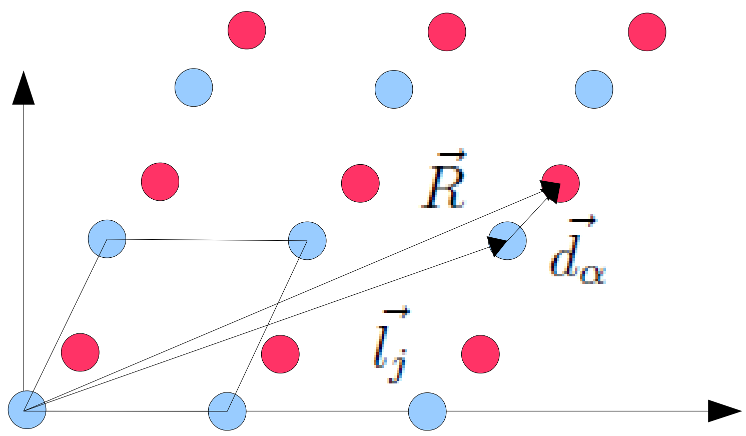
$$\frac{d\sigma}{d\Omega}_{coh.el} = N_0 \frac{(2\pi)^3}{v_0} \langle b \rangle^2 \sum_{\vec{\tau}} \delta(\vec{\kappa} - \vec{\tau})$$

- Scattering occurs when κ meets a vector of the reciprocal lattice τ
- Reciprocal lattice vectors τ are perpendicular to a corresponding lattice plane indexed by the Miller index (h,k,l) and

$$d_{(h,k,l)} = \frac{2\pi}{|\vec{\tau}_{h,k,l}|}$$

4.1 Elastic scattering from a single crystal: Structure factor

More than one atom in the unit cell: $\vec{R} = \vec{l_j} + \vec{d_\alpha}$



$\vec{l_j}$ Position of the j-th unit cell

$\vec{d_\alpha}$ Position of the α-th atom in the unit cell

$$\frac{d\sigma}{d\Omega}_{coh.el} = N_0 \frac{(2\pi)^3}{v_0} \left| \sum_{\vec{d}} b_d e^{i\vec{\kappa}\vec{d}} \right|^2 \sum_{\vec{\tau}} \delta(\vec{\kappa} - \vec{\tau})$$

$$S_{\vec{\tau}} = \sum_{\vec{d}} b_d e^{i\vec{\kappa}\vec{d}}$$

Structure factor (sum over one unit cell)

4.1 Elastic scattering from a single crystal: Thermal motion

Going from operator to standard vector notation of R_j:

➡ Neglect thermal vibration of atoms around their equilibrium position

$$2W(\vec{\kappa}) = \frac{1}{3}\kappa^2 \langle u^2 \rangle$$

Debye-Waller factor describes mean dispalcement <u²>

➡ Final result for elastic coherent scattering on crystals

$$\frac{d\sigma}{d\Omega}_{coh.el} = N_0 \frac{(2\pi)^3}{v_0} e^{-2W(\vec{\kappa})} \sum_{\vec{\tau}} |S_{\vec{\tau}}|^2 \, \delta(\vec{\kappa} - \vec{\tau})$$

Normalization — Debye-Waller — Structure factor — Bragg positions