CENTRE FOR ENERGY RESEARCH

INTRODUCTION TO NEUTRON SCATTERING

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Neutron

NEUTRON IS AN ELEMENTARY PARTICLE

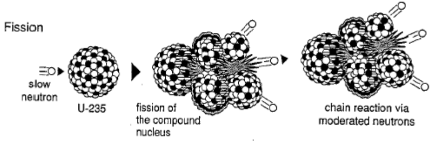
- Originated from the nuclei
- Freed by nuclear interaction
- Not stable in free form
- Interacts with nuclei / magnetic field

DATA

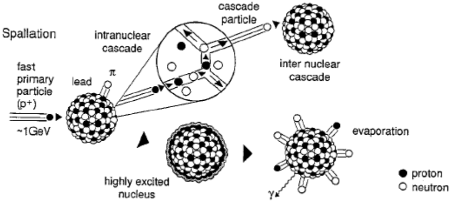
- Mass: $1.67476 \cdot 10^{-24}$ g
- Charge: 0 C
- Spin: 1/2
- Magnetic dipole moment: -1,91315 μ_n
- Half time: 882.9 s

Sources of neutrons

Fission: 3 neutron / reaction

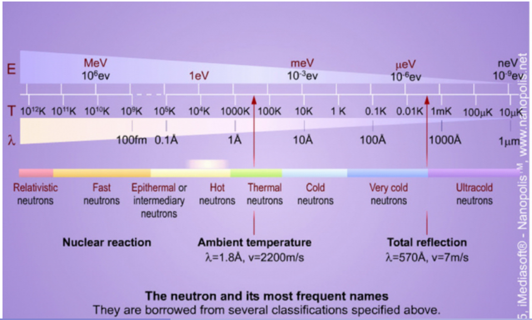


Spallation: 30 neutron / reaction



Moderations

- Hot: hot graphite
- Thermal: water, heavy water
- Cold: liquid H (orto or. para), deuterium, mesythelene..
- Ultracold: Solid deuterium

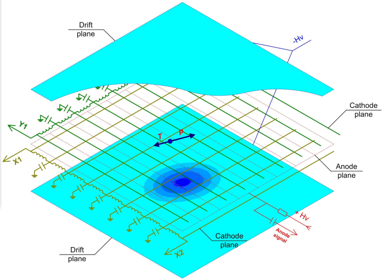


Detecting of neutrons

The energy of thermal neutrons is low

Converter is needed

- $n +^{10} B \rightarrow^{7} Li + \alpha$: BF_3 gas, solid B_4C,
- $n +^{6} Li \rightarrow^{3} H + \alpha$: ZnS:Li scintillator
- $n +^{3} He \rightarrow^{3} H + p$: ^{3}He gas
- $n + Gd \rightarrow \gamma, conversione$



Delay-line type
2D position sensitive
^{3}He detector

Detection

- Proportional chamber: electron multiplication
- Scintillator: light detectors (PEM, diodes, camera)

Properties of neutron

Particle

- mass: m_n
- velocity: v
- $E = \frac{m_n v^2}{2}$
- $p = m_n v$

Wave

- wavelength: λ -> wavenumber: $k = 2\pi / lambda$
- frequency: ν
- $E = h\nu = \hbar\omega$
- p $= \hbar k$

$$\Psi(r,t) = exp(ikr - \omega t$$

Some useful numbers:

$$\lambda = 1\text{Å(thermal)}: \; E \approx 80meV, \; v \approx 4km/s, \; f \approx 20Thz$$

$$\lambda = 4\text{Å(cold)}: \; E \approx 20meV, \; v \approx 1km/s, \; f \approx 2Thz$$

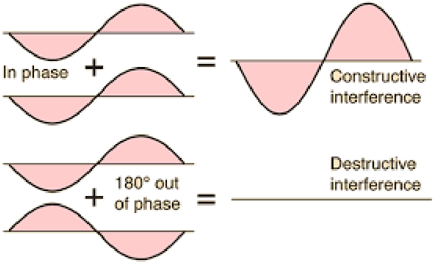
Interference

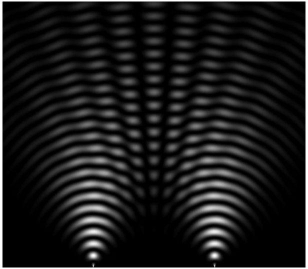
Wave

- Time period: T
- Frequency: f = 1/T
- Angular frequency: $\omega = 2\pi f$
- Wavelength: λ
- Wavenumber: k

Wave

- $\Psi = e^{i(kr-\omega t)}$
- Phase:$kr - \omega t$
- Phase difference: π: destructive interference, 2π: constructive interference





Neutron - X-ray differences

	Neutron	X-ray
Base of scattering	potential	charge oscillation
Scattering on	nucleus / magnetic field	electron density
Scattered intensity	Isotope - dependent	Z^2
Penetration depth	some cm	« mm
Energy @ 1 A	81 meV	12.4 keV
Source Brillance	Unit	10^{10} Unit
Atomic scattering factor	isotropic	decreasing in backscattering

Neutron - matter interactions

- Absorption:
  - Activation analysis (NAA, PGAA)
  - Radiography
  - Nuclear physics investigations
- Scattering
  - Elastic (Energy of neutron does not change): Investigation of static structure
  - Inelastic (Energy of neutron changes): Investigation of dynamic structure, excitation in condensed matter

The interactions are measured with cross section

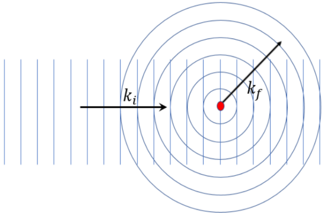
- Microscopic cross section (nucleus): σ [barn=10^{-24} cm^2]:
  Number of interactions within a secundum pro unit intensity
- Macroscopic cross section (matter): $\Sigma = n\bar{\sigma}$ [1/cm] (sample)
  where n [1/cm^3] is the nuclear density
  Number of interactions within a secundum pro unit intensity and unit volume of the sample

Scattering

The nuclei scatter the thermal neutrons in spherical wave

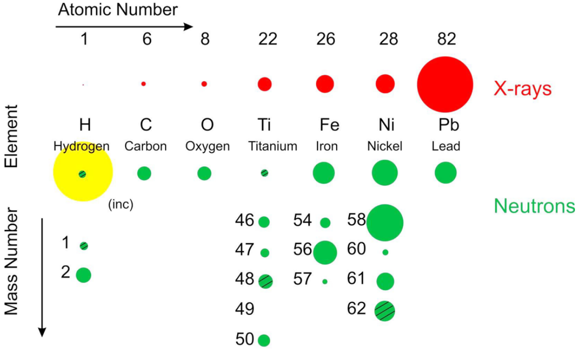
- Short range interaction (fm)
- The scattering is described by b (in fm units):
  b: The scattered amplitude over the amplitude of the incident wave (In the case of X-rays the scattering is anisotropic due to the size of the electronic shell)
- The scattered intensity is given by the scattering cross section: $\sigma_s = 4\pi b^2$

Note that b can be negative, and it can be complex if the nucleus is a high absorber



Scattering amplitudes (X-ray and Neutron)

- Neutron: Isotope sensitivity, non monotonic function of the elemental number. Isotropic
- X-ray: scattered by the electronic density: ($b \approx c\cdot$ elemental number). Anisotropic



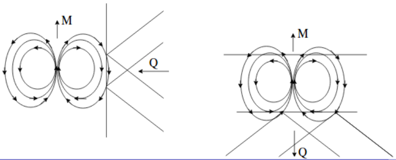
The diameters of the circles shown scale with the scattering amplitude $f_x(\sin\Theta=0)$ for x rays, and b_{coh}*10 for neutrons. Hatching indicates negative scattering amplitudes.

Scattering on the magnetic field

Effect of the magnetic field

- The component of the magnetic field parallel with the neutron spin gives an extra potential field
- The component of the magnetic field perpendicular to the neutron spin causes a spin-flip
- Magnetic scattering factor:
  $f_m(\mathbf{q}) = F(q)s_n(\mathbf{e}(\mathbf{eh}) - \mathbf{h})$, $e = |q|/q$, h: spin of the atom

scattering on magnetic atom is not isotropic (like X-ray scattering):
Polarization factor: $\mathbf{e}((\mathbf{eh}) - \mathbf{h})$
magnetic form factor: $F(q)$



Kinematic Scattering Theory

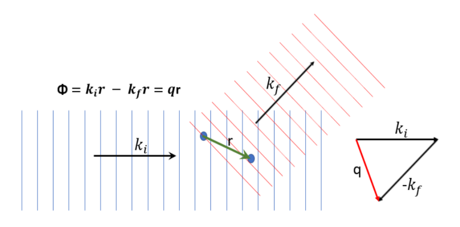
Gives a simplified model for the scattering on condensed matter

The wave is scattered only once and leaves the sample

Not applicable to diffraction on perfect crystals and reflectometry

Scattering on atomic structures

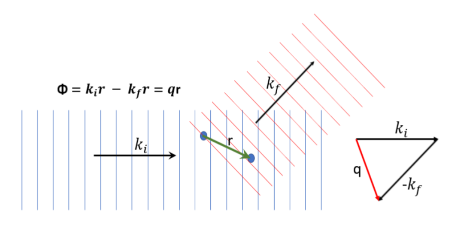
The spherical wave is close to plane wave at large distances



- Only the phase differences are important at the detector: $k_i r - k_f r = qr$
- The scattered intensity is measured as a function of q (reciprocal space)
- The scattered intensity: $|\Psi(\overrightarrow{q})|^2$

Scattering on atomic structures

Changing to scattering length density: $\rho(\vec{r}) = \frac{\Sigma b}{V}$



If we step with π/q steps, the intensity shows how many times we have to step up and down

- large-q: small steps, we see the grass (atomic resolution)
- small q: large steps, we see the haystack (nano objects)

Scattering on atomic structures

If we step with π/q steps, the intensity shows how many times we have to step up and down

Large-q: small steps, we see the grass (atomic resolution)
Small q: large steps, we see the haystack (nano objects)

- Large steps (small q, small angle scattering): we do not see the grass (the atoms)
- Small steps (large q, diffraction): we do not see the haystack (nanosized particles)
- Haystacks on the top of the mountain (steps up and down but at large altitude) the signal is the same: Contrast give the intensity
- Random landscape: at every step size we can step up and down
  Intensity is constant: incoherent scattering

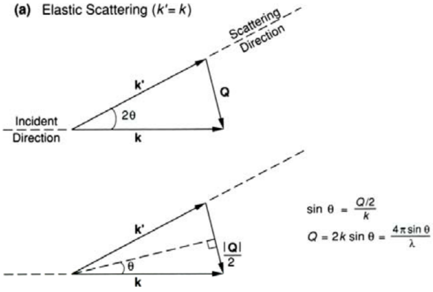
Elastic scattering

No energy change
more than 99% of the scattering events in solid samples

Incident and scattered wavenumbers are the same

Static structure

- Diffraction
- Small angle scattering
- Reflectometry



The scattered intensity depends only on q:

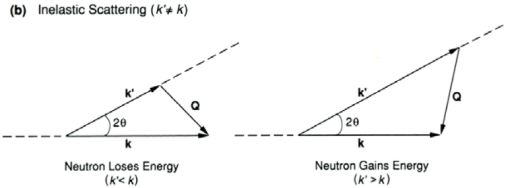
$$\vec{q} = \vec{k}_f - \vec{k}_i$$
$$q = 2k\sin(\theta)$$

Inelastic scattering

The energy of neutrons change during scattering

Dynamic structure
(molecular vibration, lattice vibration, diffusien etc..)

- Three axis spectrometer
- Indirect - direct TOF
- Backscattering
- Neutron spinecho



The scattered intensity depends on the momentum and energy transfer:

$$\vec{q} = \vec{k}_f - \vec{k}_i$$

$$E = E_f - E_i$$

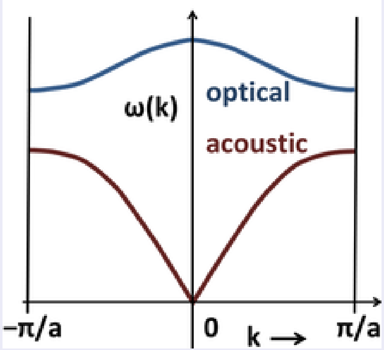
Weak intensity in solid samples

Scattering on moving atomic structures

Example: oscillations (phonons)

Oscillation has momentum and energy (quasy - particle)

Signal is q- and ω dependent



A little mathematics

- Scattered wave function is the Fourier transform of the sample
- We see the Intensity: $\Psi\Psi^*$
- Convolution theory: $\mathcal{F}(fg) = F * G$ $\mathcal{F}(f * g) = FG$:
  - Van - Hove rule: Scattered intensity is the Fourier-transform of the autocorrelation function of the sample $I = \mathcal{F} < \rho, \rho >$
  - Structure factor (unit cell $*$ lattice
  - Debeye - Waller effect (lattice $*$ atomic movement) $<->$ Small crystallites (lattice multiplied by distribution function
- Random change: $< \rho, \rho >= \delta(r) \rightarrow I(q) = C$
- Contrast: $< \rho, \rho >= C+ < \delta\rho, \delta\rho >\rightarrow I = \delta(q) + \mathcal{F} < \delta\rho, \delta\rho >$

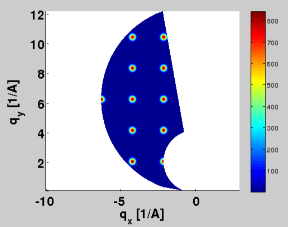
Properties of scattering function

- Infinite lattice gives infinite latice in q
  Just with a strictly given steps gives the same up-down series
- Gaussian-like particle gives Gaussian-like particle
- Inverse relation: larger particle gives signal on small q, smaller particle gives signal at large q
- Complex system: particles at different point (convolution) gives the production of the signal of particles and the signal of positions
- Vice-versa: scattering objects in finite-range (product): gives the signal of centers smeared with the signal of scattering objects (convolution)

Scattering on atomic structures

Example: Diffraction on a single crystal with d lattice spacing

- We need the exact step size to see signal
- Two times - three times ... smaller steps give the same signal (up down same, same up down...)



Simulated diffraction image of a cubic crystal using TOF diffraction

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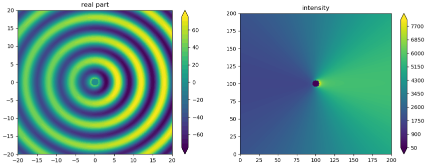
Larger particles

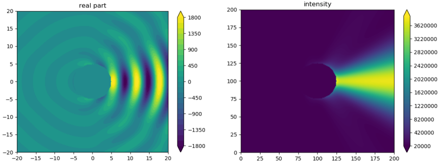
Example: Larger particles (magnetic scattering, X-ray scattering)

If particle size is comparable to the wavelength, the intensity decreases in backward scattering (e.g. X-ray scattering factor)



Example: Large particles (nanoparticles)

If the particle larger than the wavelength, one cannot see the structure of the particle only it's shape (Small Angle Scattering)



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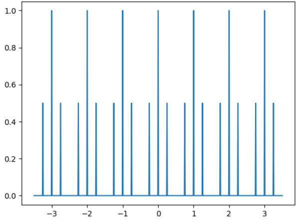
Properties of scattering function: structure factor

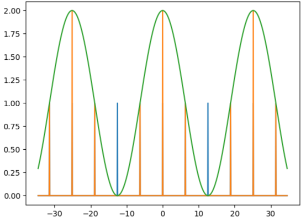
for crystals: L is a lattice U shows the heights of peaks of L:

$|F(hkl)|^2$: Structure factor



Real space

$\longrightarrow$



Reciprocal space

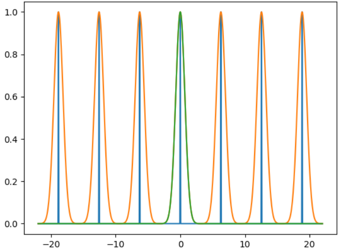
Properties of scattering function

- Infinite lattice gives infinite latice in q
  Just with a strictly given steps gives the same up-down series
- Gaussian-like particle gives Gaussian-like particle
- Inverse relation: larger particle gives signal on small q, smaller particle gives signal at large q
- Complex system: particles at different point (convolution) gives the production of the signal of particles and the signal of positions
- Vice-versa: scattering objects in finite-range (product): gives the signal of centers smeared with the signal of scattering objects (convolution)

Properties of scattering function: non-ideal systems

Use of convolution theorem

- Thermal motion: atomic positions are convoluted with a gaussian: peaks at large q are decreased: Debeye Waller effect
- The finite size of a periodic system (e.g. nanocristallites) infinite lattice is multiplied with the size distribution function:
  Scherrer equation: The width of the peak is: $w = \frac{1}{d}$, d: size of cristallites, k$\approx$ 1 is the shape factor

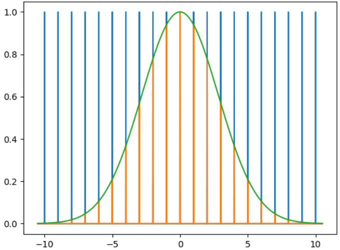


Debye - Waller

$\longrightarrow$

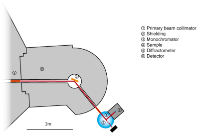
$\longleftarrow$

Scherrer



Instrumentation: Monochromators

Single crystal

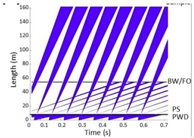


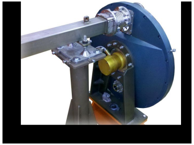
Heidi diffraktométer Garching

- Pyrolithic graphite
- Si, Ge
- Copper
- Nickel
- ...

Resolution $\Delta\lambda = 0.1 - 4\%$

Time of flight (TOF)





Choppers

Resolution: flexible ($\Delta\lambda = C$)

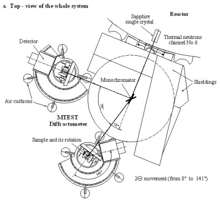
Velocity selection

Mechanical velocity selector

$\frac{\Delta\lambda}{\lambda} = 10\% - 20\%$

Some examples: Elastic instruments

Monochromatic crystal diffractometer

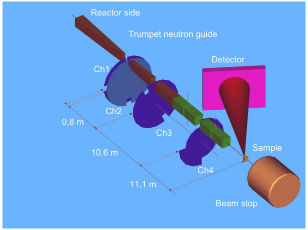


Mtest diffractometer

- Monochromator
- Moving sample-table to change wavelength
- Moving detector to change angular range

Time of flight (TOF)

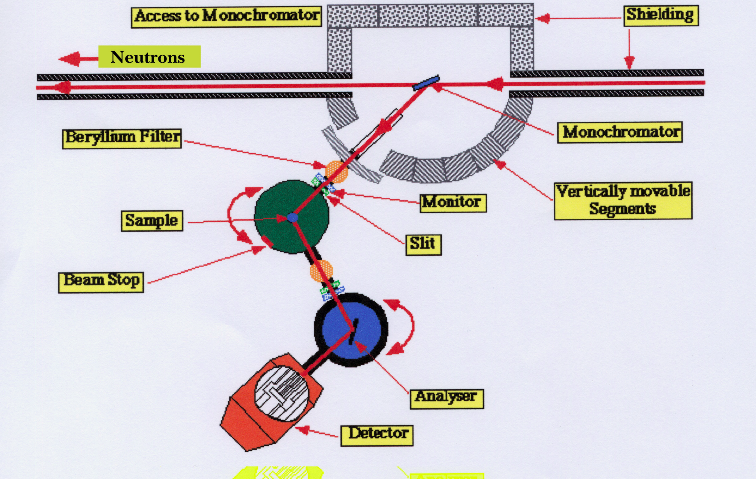
Diffractometer



- Chopper produces pulses
- Large wavelength band
- Measurement mostly in one setup

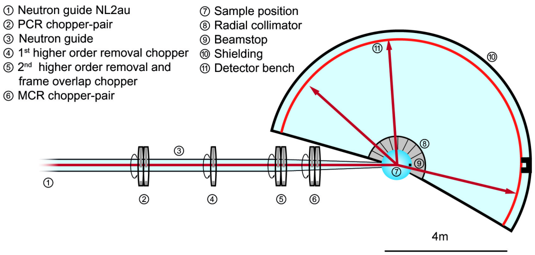
Some examples: Three Axis Spectrometer

Three axis spectrometer

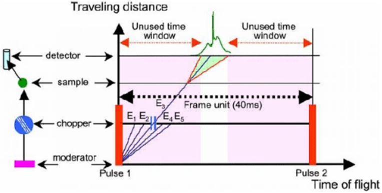


(crystal - crystal)

Some examples: Direct TOF spectrometer



- Monochromatic beam
  - TOF
  - Monochromator
- Chopper at sample
- Time of flight from the sample to the detector



Thank you for attention

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