Physics with Neutrons I

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Exercise sheet 7 https://wiki.mlz-garching.de/n-lecture06:index

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Solutions

1. Imaging Basics

In neutron imaging, the transmission of neutrons through a sample is determined, which can be used to distinguish between different materials. In many experiments it is sufficient only to consider the neutron absorption in a material. However, there are other cases where this is completely wrong. One prominent example is the comparison between water (hydrogen) and iron. The respective absorption cross sections are: $\sigma_{abs}^{H} = 0.333$barn, $\sigma_{abs}^{Fe} = 2.56$barn (for thermal neutrons). In measurements, though, water clearly shows a stronger neutron attenuation. What other factors besides absorption have to be considered? What are their impact on an imaging experiment?

Solution

Besides absorption, the neutron transmission also depends on the scattering properties of a material. Incoherent scattering deflects neutrons in arbitrary directions which results in a homogeneous background of neutrons. In an experiment, this effect will reduce transmission, as the detector only covers a small solid angle. Additionally, the absolute noise level and the signal to noise ratio will increase, due to the scattered neutrons arriving at the detector. Coherent scattering (i.e. bragg scattering) is inhomogeneous and results in lower transmission, if the neutrons are scattered under large angles (so they wont hit the detector) or in increased intensity at certain pints on the detector for small scattering angles. Especially at sample edges or material interfaces, artifacts can happen due to coherent scattering.
The list below gives values for three different materials. Even though σ_{abs} is significantly larger for Fe compared to H, the attenuation of H is higher due to the incoherent scattering. additionally it becomes clear why for water, the oxygen is usually ignored, as both absorption and incoherent scattering are negligible.

Element	$\sigma_{coh}(barn)$	$\sigma_{inc}(barn)$	$\sigma_{abs}(barn)$
H	1.76	80.3	0.333
O	4.23	0.0008	0.00019
Fe	11.2	0.4	2.56

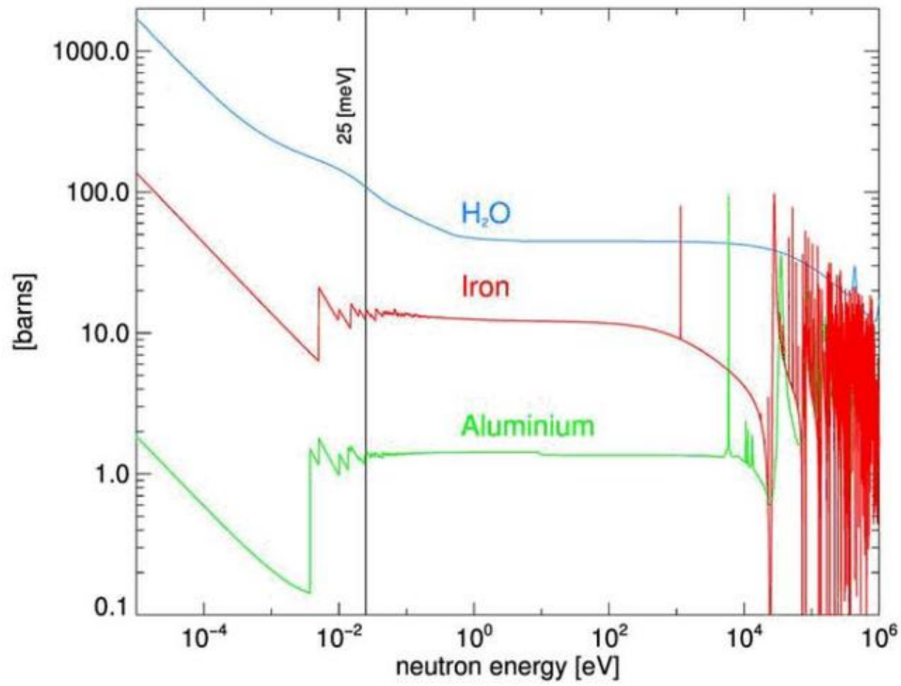
2. Bragg-Imaging

Neutron interaction with matter is generally energy dependent. Scattering and absorption typically increase with increasing neutron wavelength.

- What does this mean for the samples used in an experiment?
- Despite neutrons passing through the sample, the measurement results might be different if we rotate the sample by 180°. What is causing this discrepancy? (Hint: the effect is strongest if we use a broad spectrum of neutrons)

Beside the general trend of neutron attenuation (see Figure below) there might appear sudden jumps at certain energies, which are caused by coherent scattering. These features are used in Bragg imaging, by taking measurements with neutrons slightly above and below a jump energy and comparing the results.

- Why are there no features in the Water curve?
- What is determining the lowest Energy of such a jump. (Hint: it's called Bragg imaging)
- Calculate the lowest jump energy for iron.



Solution

- By changing the neutron wavelength on fan experiment, the transmission of a sample can be tuned to best fit the measurement. For small objects, longer wavelengths have to be used than for large object. Otherwise, the image might show no (measurable) attenuation at all, or the transmission drops to zero.
- Neutrons with different wavelengths interact differently with matter. Low energy neutrons generally get absorbed or scattered more easily, so the front part of a larger sample has a larger impact on them, compared to high energy neutrons. Accordingly, the back part of the sample will see a neutron beam with a different spectrum (shifted to higher energies). This Effect is known as beam hardening, and is for example important for tomographies of inhomogeneous or complex samples, where in a full rotation of a sample, two images rotated by 180°might not be identical.
- Water has a comparatively large cross section due to the large incoherent scattering of hydrogen (which varies smoothly with energy). The additional features in Iron are caused by coherent scattering, when the Bragg condition is fulfilled. In water, coherent scattering is low in the first place but more importantly, it is a liquid and has no periodic structure which might cause Bragg Scattering.
- The lowest feature is the first instance of the Bragg condition being fulfilled. Neutrons are scattered in a certain direction and are lost to the transmitted beam. Be ware, that in

experiment, there is a huge difference between single crystals and polycrystallin samples, as for the former not only the energy but also the orientation has to match the Bragg condition.

- Iron (under ambient conditions) has a BCC crystal structure with lattice parameter $a = 2.87$Å. For the lowest energy Bragg peak we take a look at the reciprocal lattice, which is an FCC lattice. By calculating the reciprocal lattice vectors we obtain the reciprocal lattice parameter $g = 2 * \pi/a = 2.19/$Å. However, this is not the correct parameter for the FCC lattice, because the unit cell of the real space BCC lattice can only extinguish Bragg peaks, not create new ones.
  The selection rules for a BCC lattice state that $h + k + l$ has to be even so the lowest peak is the (110)-Peak with $q = 3.10/$Å. The first instance for reaching this reciprocal lattice point is for $k_i = k_f = q/2$ and accordingly $\lambda = 2\pi/k_i = 4.06$Å. This is the lowest neutron energy which fulfills any Bragg condition in iron ($E = h^2/(2m\lambda^2) = 4.97$meV)

3. Patterson Function

Probably the biggest problem in all scattering experiments is the phase problem: we can only measure the scattering intensity (which is real) instead of the scattering function (which is complex). A way of getting around this problem is the Patterson function which is defined by the Fourier transform of the scattering Intensity:

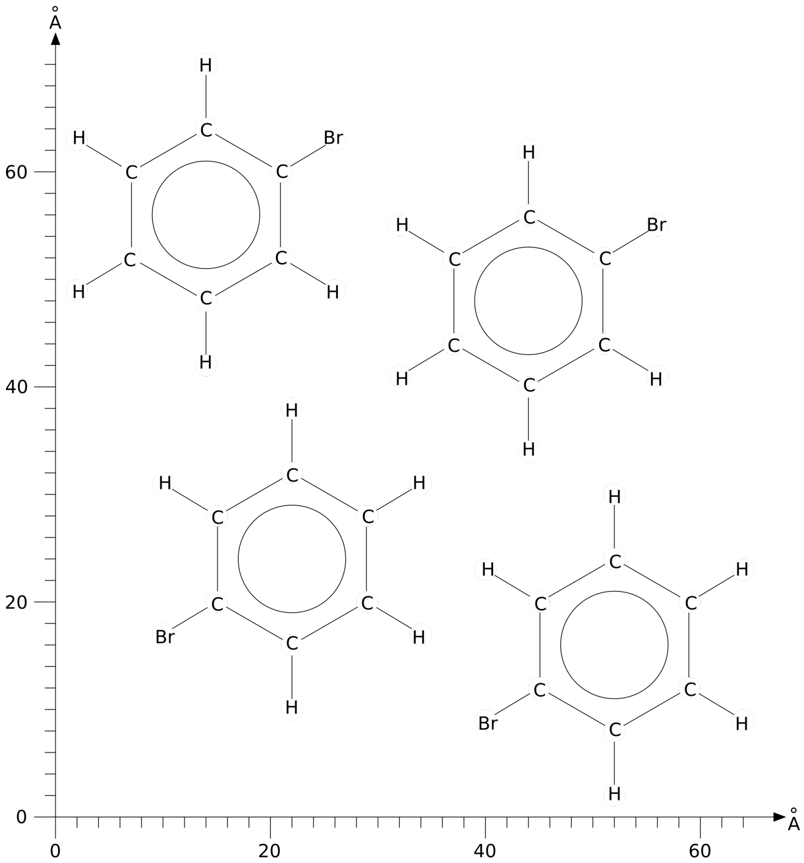
$$P(\vec{r}) = FT\left(I(\vec{q})\right)$$

which can be obtained by experiment.
The equivalent definition in real space is given by the self correlation of the crystal structure:

$$P(\vec{r}) = \rho(\vec{r}) \otimes \rho(\vec{-r})$$

where ρ is the scattering length density (or electron density in case of X-rays).

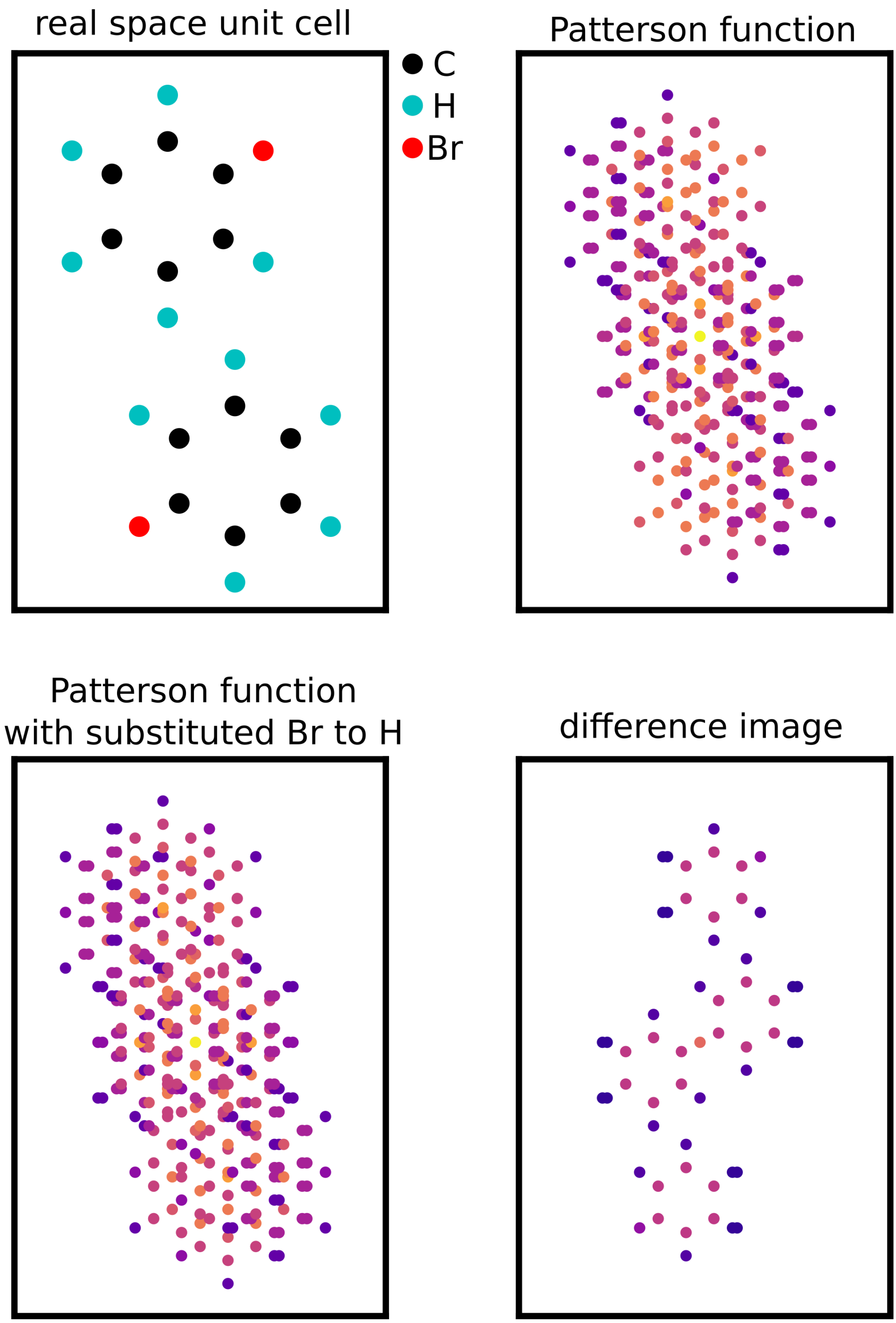
Shown below is a possible structure of a brombenzene crystal, which will be used to test the Patterson method from a real space perspective


Å
60
40
20
0
0
20
40
60
Å
H
C
Br

- Choose a unit cell.
- Calculate (compute) the Patterson function for the unit cell (take the positions from the image and assume point like atoms).
- Interpretation of a Patterson function becomes very much easier if one can obtain it for nearly identical crystals by comparing them to each other. Assume a substitution of Br by H (which does noch change the crystal structure) and calculate the Patterson function again.
- Instead of the atomic substitution, could the effect used in Bragg edge imaging be used to change the scattering cross section of one specific atom in the crystal?
- Subtract one Patterson function from the other and interpret the result.

Solution

- There are two different positions of the bromium, so a unit cell consists of two brombenzene molecules, e.g. the top left and bottom left ones. In the first panel of the image below, different atoms are coded by different colors.
- We use the second method (the convolution) to compute the Patterson function. In practice this means that we place a copy of the unit cell on each of its atoms, multiplied by the corresponding scattering cross section. the color coding of the other three panels gives the magnitude of the Patterson function (dark/violet is a low value, light/yellow is a high value)
- We repeat the calculation for the unitcell with replaced Br atom and get a Patterson function which has the same pattern as before, but has some different intensities.
- after the subtraction, only those parts remain that were caused by the change of Br to H. Essentially we see a convolution of the unit cell onto both positions of the bromium atom, which is why we see the unit cell twice. There are some double points visible, which are an artifact due to the method of calculation (basically a rounding error).


real space unit cell
C
H
Br
Patterson function
Patterson function
with substituted Br to H
difference image