Physics with Neutrons I

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Exercise sheet 6 https://wiki.mlz-garching.de/n-lecture06:index

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1. Instrument Resolution I

For neutron scattering experiments, atoms can be well described by delta functions. We have seen so far, that Bragg scattering from a perfect (ans sufficiently large) single crystal gives rise to very sharp intensity peaks which are again well described by delta functions. However, in experiment these sharp peaks always have a finite width and have the shape of peak functions (such as Gaussian or Lorentzian distribution). This is no effect of real samples, but of the experimental setup. the two main contributions to this broadening are:

- the incident beam direction. A neutron beam is never perfectly parallel, but has a finite divergence.
- the neutron wavelength. Both, monochromators and velocity selectors let through a certain spectrum of neutrons.

Consider a 1D experiment where we look at scattering under small angles. The incident neutron beam is collimated in a 20m long flight tube with 10mm diameter apertures and the wavelength is determined by a velocity selector. The selector has a triangular shaped spectrum with $\delta\lambda/\lambda = 5\%$ (i.e. the FWHM of the distribution has the calue of $\delta\lambda$).

- For incoming neutrons, what is the shape and width of the angular distribution?
- How do angular and wavelength spread affect the scattering process?
- What is the shape and width of Bragg peaks finally observed?
- What changes if we consider scattering under large angles?
- Think about other possible factors influencing the shape of Bragg peaks in an experiment!

2. Instrument Resolution II

Insulating organo-metallic compound $NiCl_2 - 4SC(NH_2)_2$ (know as DTN) demonstrates magnetoelastic properties (Phys. Rev. B 77, 020404(R) (2008)). In an applied magnetic field its c-axis first shrinks by $6 \cdot 10^{-3}\%$ and then expands up to $2.2 \cdot 1^{-2}\%$ in comparison to the zero field value. Calculate whether it is possible to detect such a change in length of the c-axis using powder neutron diffractometer HRPT located in PSI (the instrumental resolution is equal to $\Delta\theta/\theta = 9.5 \cdot 10^{-4}$ for $Q = (002)$. The unit cell is tetragonal (space group I4 number 79) and the lattice parameters (zero magnetic field) are: $a = b = 9.558$ Å, $c = 8.981$ Å.

3. Towards disordered systems

As the lecture will now go from Well ordered crystals to liquids and other disordered systems, take some time to play around with disorder in 1D atomic chains. Similar to the computations in exercise 3 on sheet 3, try out some different kinds of disorder:

- different atoms (with different scattering length) in perfect order, complete disorder.
- substitutional defects can be modeled by adding a small chance to have the wrong atom at each lattice point
- imperfect ordering can be introduced by adding a small random shift to each lattice position. this can be either individual for each atomic position, or cumulative.
- some binary alloys tend to cluster. this can be modeled by selecting the Atom for each lattice position randomly, but make it dependent on the previous position with a bias towards the same kind of atom.

This is no exercise with a fixed solution. It is rather meant to illustrate the effects of different kinds of disorder in crystals and how strong they are. Remember to compare them to scattering from liquids, once they are covered in the lecture!
If you have trouble implementing an idea in python, feel free to write me an email.