Physics with Neutrons I

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Exercise sheet 5 https://wiki.mlz-garching.de/n-lecture06:index

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1. Structure Factor of the Diamond Lattice

The Diamond lattice is defined as a FCC lattice with a basis of two identical atoms at vectors $(0, 0, 0)$ and $(4/d, 4/d, 4/d)$ (with d the lattice spacing). Determine the positions of all atoms in one unit cell and calculate the structure factor of the diamond lattice, which is defined by

$$F(k = \vec{G}_{hkl}) = \sum_{unitcell} exp(-i\vec{G}_{hkl}R_j)$$

with $\vec{G}_{hkl}$ the reciprocal lattice vectors and R_j the atoms in a unit cell. Formulate rules for the dependence of $F(k = \vec{G}_{hkl})$ on the h, k, l.

2. Powder Diffraction and Selection Rules

In a powder diffraction experiment with a material having a cubic unit cell und using neutrons with a wavelength $\lambda = 1.5$Å , the first few Bragg Peaks occur at the scattering angles $\vartheta = 43.31°$, 50.44°, 74.12°, 89.93°. Determine the structure (sc, fcc, bcc, etc.) these peaks correspond to. Based on the information draw the reciprocal lattice with the allowed and forbidden Bragg peaks in the (hk0) and the (hhl) plane. draw the same reciprocal lattice planes for a diamond lattice.

3. The Lorentz Factor

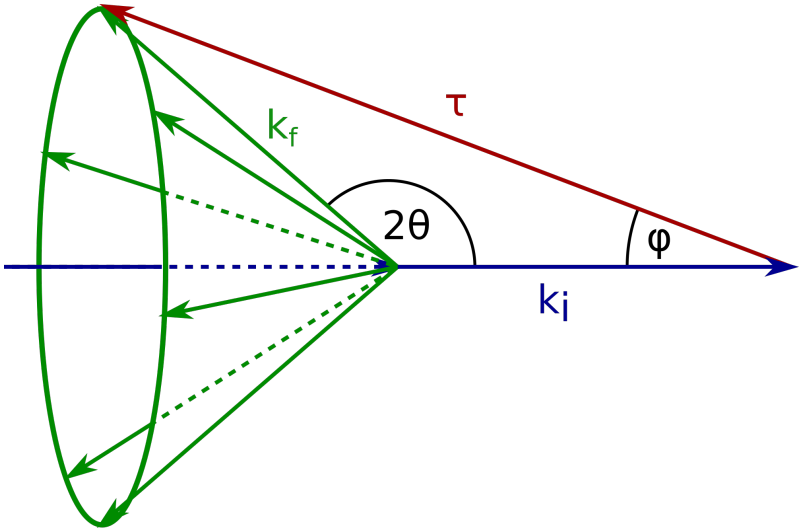
For Polycrystals or in powder diffraction experiments, the measured intensity has to be corrected for a geometrical factor called the Lorentz factor :

$$L(\theta) = \frac{1}{sin(\theta)sin(2\theta)}$$

The origin for this factor is twofold:

- The statistical distribution of crystal orientations has to be considered. (What fraction of the sample contributes to scattering?)
- The detector covers only a part of the Debye-Scherrer cone, which describes Bragg scattering from a polycrystalline sample. As sketched below, for a given Bragg reflex, the scattered wave vector k_f can be rotated freely around the incident neutron Beam k_i. (this is again due to the random distribution of crystal orientations)

Derive the Lorentz factor.
The derivation will include some experimental quantities (like the lattice parameter) which can be dropped at the end.


τ
k_f
2θ
φ
k_i