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 $(d/4,d/4,d/4)$ (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

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

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.

Solution

All atomic positions to consider in a Diomond Lattice are those of a FCC lattice:

$$(0,0,0)\ ,\ (\frac{d}{2},\frac{d}{2},0)\ ,\ (0,\frac{d}{2},\frac{d}{2})\ ,\ (\frac{d}{2},0,\frac{d}{2})$$

and those of the second atom of the basis, which are shiftet by $(d/4,d/4,d/4)$:

$$(\frac{d}{4},\frac{d}{4},\frac{d}{4})\ ,\ (\frac{3d}{4},\frac{3d}{4},\frac{d}{4})\ ,\ (\frac{d}{4},\frac{3d}{4},\frac{3d}{4})\ ,\ (\frac{3d}{4},\frac{d}{4},\frac{3d}{4})$$

The structure factor is the Fourier transform of the real space unit cell, evaluated at all Bragg peak positions of the cubic crystal. The reciprocal lattice vectors are $\vec{G}_{hkl} = h\vec{p_x} + k\vec{p_y} + l\vec{p_z}$, with the reciprocal unit vectors $\vec{p}$

$$\vec{p_x} = \frac{2\pi}{d}(1,0,0)\ ,\ \vec{p_x} = \frac{2\pi}{d}(0,1,0)\ ,\ \vec{p_x} = \frac{2\pi}{d}(0,0,1)$$

Inserting this gives:

$$\begin{aligned}
F(\vec{k}=\vec{G}_{hkl}) &= \sum_{unitcell} exp(-i\vec{G}_{hkl}\vec{R}_j) \\
&= e^{(-i0)} + e^{(-i\pi(h+k))} + e^{(-i\pi(k+l))} + e^{(-i\pi(h+l))} \\
&+ e^{(-i\frac{\pi}{2}(h+k+l))} + e^{(-i\frac{\pi}{2}(3h+3k+l))} + e^{(-i\frac{\pi}{2}(h+3k+3l))} + e^{(-i\frac{\pi}{2}(3h+k+3l))} \\
&= 1 + (-1)^{h+k} + (-1)^{k+l} + (-1)^{h+l} + (-i)^{h+k+l} + (-i)^{3h+3k+l} + (-i)^{h+3k+3l} + (-i)^{3h+k+3l} \\
&= \left[1 + (-1)^{h+k} + (-1)^{k+l} + (-1)^{h+l} + (-i)^{h+k+l}\right]\left[1 + (-i)^{h+k+l}\right]
\end{aligned}$$

This result includes the form factor of the FCC lattice (if we drop $(-i)$-part in the second bracket) which equals 4 for h, k, l all even or all odd and zero else. With the additional term from the two-atom basis the result is:

- 0 if h, k, l not all even or not all odd
- 8 if h, k, l all even and $h + k + l$ divisible by 4
- 0 if h, k, l all even and $h + k + l$ not divisible by 4
- $4(1 \pm i)$ if h, k, l all odd (we don't distinguish this, because the absolute value is the same)

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.

Solution

First of all, we can calculate the lattice plane distances $d_i = d_{hkl}$ from the given angles ϑ by using the Bragg equation

$$d_i = \frac{\lambda}{2} \sin\left(\frac{\vartheta}{2}\right)$$

Which results in $d1 = 2.0323$Å, $d2 = 1.7600$Å, $d3 = 1.2445$Å, $d4 = 1.0613$Å.
in a cubic unit cell, the plane distances are related to the lattice constant and the Miller indices by the following relation (which is essentially the Pythagorean theorem)

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

We will now look at the first four allowed reflexes in sc, bcc, fcc lattices and determine, if the observed reflexed could have been fit the crystal structure.

- simple cubic: all combinations of hkl are allowed

reflex	d_{hkl}	a [Å]	
100	a	2.0323	→ no match
110	$a/\sqrt{2}$	2.489	
111	$a/\sqrt{3}$	2.1555	
200	$a/2$	2.1226	

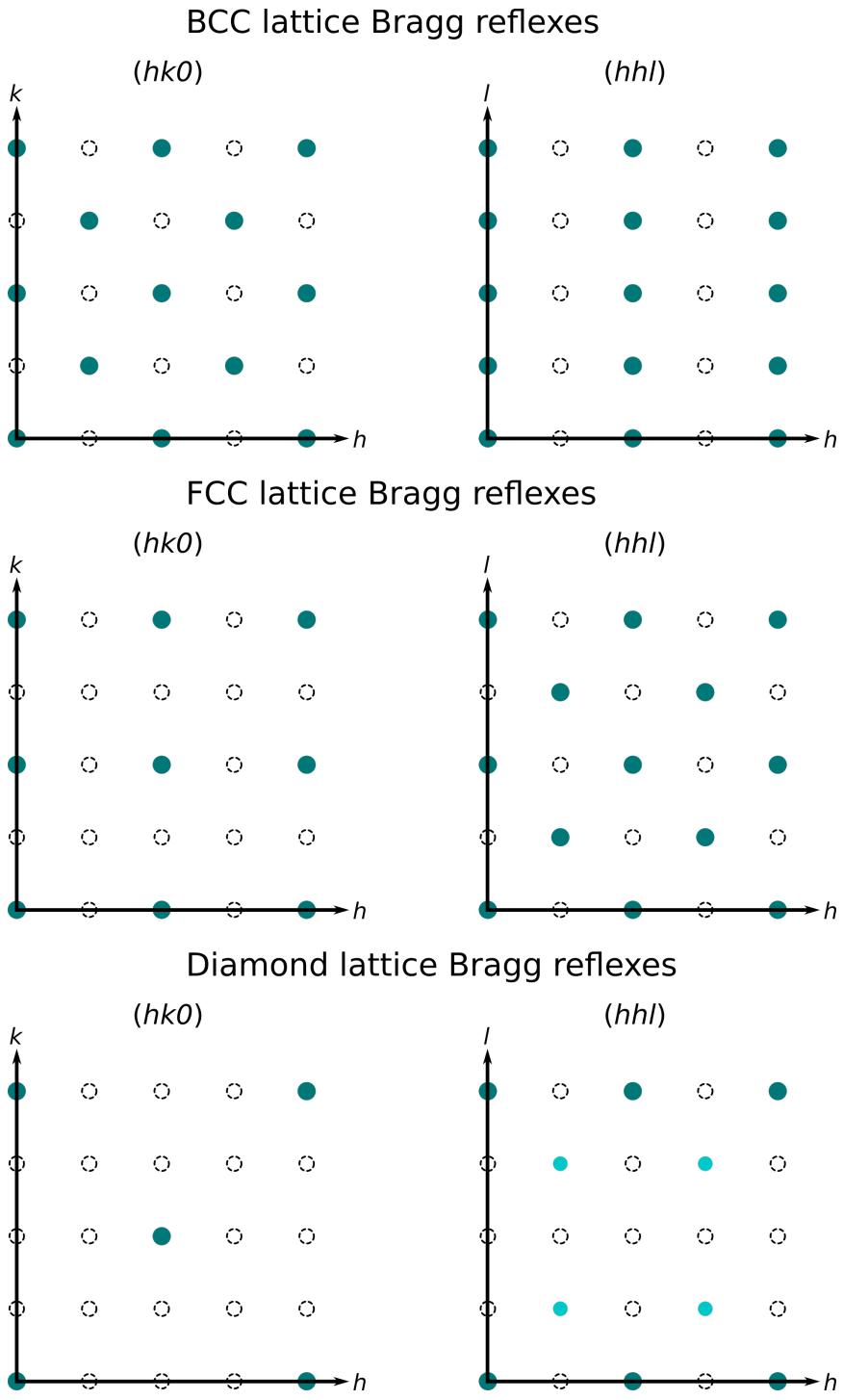
- body centered cubic: $h + k + l$ have to be even

reflex	d_{hkl}	a [Å]	
110	$a/\sqrt{2}$	2.874	
200	$a/2$	3.52	→ no match
211	$a/\sqrt{6}$	3.048	
220	$a/\sqrt{8}$	3.002	

- face centered cubic: hkl have to be all even or all odd

reflex	d_{hkl}	a [Å]	
111	$a\sqrt{3}$	3.52	
200	$a/2$	3.52	
220	$a/\sqrt{8}$	3.5199	
311	$a/\sqrt{11}$	3.5199	$\rightarrow$ match!

The structure is face centered cubic with a lattice constant of $a = 3.52$Å. (this matches elemental nickel)



3. The Lorentz Factor

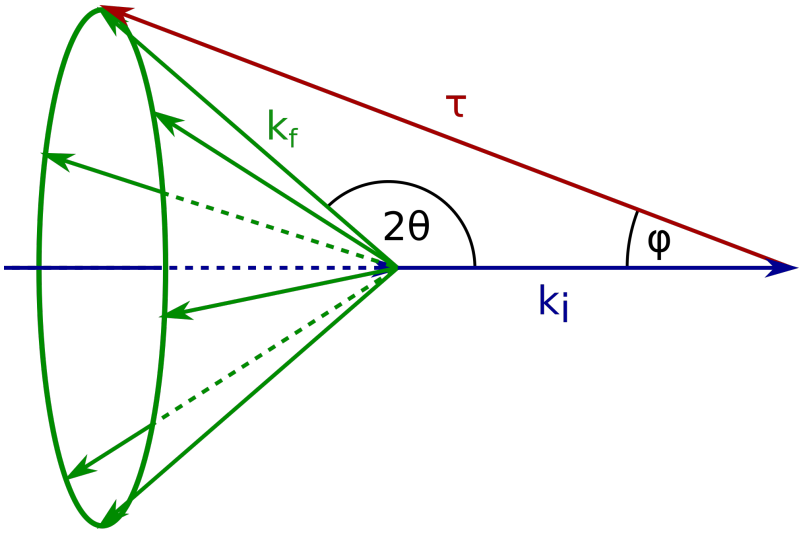
For Polycrystals or in powder diffraction experiments, the measured intensity has to be corrected for a geometrical factor called the Lorentz factor :

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

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.



Solution

First we consider the statistical distribution of the crystallites in a polycrystalline sample or powder. In order to contribute to Bragg scattering, a crystallite must contain an appropriate reciprocal lattice vector $\vec{\tau}$. For a polycrystall, all crystallites have the same set of reciprocal lattice vectors, but their lattices are oriented isotropically in space. The geometry of this problem is shown below, where all possible orientations of $\vec{tau}$ lie on the surface of a sphere. Our task is to select the area fraction of this sphere that contributes to our measurement

We start by reducing the 3D to a 2D problem by evaluation the rotational symmetry around the incident beam. The area in a certain direction (shaded area) is then given by:

$$2\pi\tau^2 \cos\theta d\theta / 4\pi\tau^2$$

The whole surface contains elastic and inelastic scattering, hence, we need to select just the area where scattering is elastic, i.e. $k' = k$. This is implemented by integration:

$$\int_0^{\pi/2} \delta(k' - k) cos\theta d\theta$$

where all constants defining the experiment have been dropped as only the θ-dependence is of interest. We can rephrase the argument of the delta function in terms of θ by using the geometry shown above:

$$k'^2 - k^2 = \tau^2 - 2\tau k\cos\phi = \tau^2 - 2\tau k\sin\theta = (k'+k)(k'-k),$$

where we used the relation $\theta = \pi/2 - \phi$, which is true for $k' = k$. Setting $k' \approx k$ yields:

$$k' - k = \frac{1}{2k}(\tau^2 - 2\tau k\sin\theta)$$

Using this result in the delta function we can perform the integration with a simple variable transformation:

$$\int_0^{\pi/2} \delta(\tau^2 - 2\tau k\sin\theta)\cos\theta d\theta.$$

$$x = 2\tau k\sin\theta \rightarrow \cos\theta d\theta = \frac{dx}{2\tau k}$$

$$\int_0^{\pi/2} \delta(\tau^2 - x)\frac{1}{2\tau k}dx = \frac{1}{2\tau k}.$$

Setting $\tau = 2k\sin\theta$ from Bragg's law we find the Angular dependence:

$$\frac{1}{\sin\theta}$$

Now we have to consider the neutron detector. It has a diameter d and a distance r from the sample. Hence it can only intercept a fraction of the scattering cone given by

$$q = d/2\pi r\sin(2\theta)$$

Again, dropping everything but the θ-dependence, we arrive at the Lorentz-Factor by multiplying both contributions:

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