
Physics with neutrons 1

Sebastian Mühlbauer, sebastian.muehlbauer@frm2.tum.de

Winter semester 2015/16

Exercise sheet 6

Due 2015–Nov–27

Lukas Karge, lukas.karge@frm2.tum.de, Tel.: 089-289-11774

EXERCISE 6.1

Prove the lattice sum equation:

$$\sum_{\mathbf{v}_{mnp}} \exp(i\mathbf{Q} \cdot \mathbf{v}_{mnp}) = \frac{(2\pi)^3}{V_{UC}} \sum_{\mathbf{G}_{hkl}} \delta(\mathbf{Q} - \mathbf{G}_{hkl})$$

Solution. Let $\mathbf{v} = m\mathbf{a}_1 + n\mathbf{a}_2 + p\mathbf{a}_3$ be a lattice vector in real space and $\mathbf{G} = h\mathbf{a}_1^* + k\mathbf{a}_2^* + l\mathbf{a}_3^*$ a reciprocal lattice vector, with m, n, p, h, k, l integer. Also let $\mathbf{Q} = q\mathbf{a}_1^* + r\mathbf{a}_2^* + s\mathbf{a}_3^*$ be an arbitrary scattering vector. Now we can write the left hand side of the equation as

$$\sum_{m,n,p} \exp(i\mathbf{Q} \cdot \mathbf{v}) = \sum_{m,n,p} \exp(2\pi i(qm + rn + sp))$$

(using $\mathbf{a}_i^* \cdot \mathbf{a}_j = 2\pi\delta_{ij}$, the defining relation of the reciprocal lattice vectors).

This sum can further be separated in three parts:

$$\left(\sum_m e^{2\pi i q m} \right) \left(\sum_n e^{2\pi i r n} \right) \left(\sum_p e^{2\pi i s p} \right),$$

of which we now only look at the first. Assume that the crystal has N (without loss of generality we set N odd) unit cells in the direction of \mathbf{a}_1 . Then the sum becomes

$$\sum_{m=-(N-1)/2}^{(N-1)/2} e^{2\pi i q m} = \sum_{m=0}^{(N-1)/2} e^{2\pi i q m} + \sum_{m=0}^{(N-1)/2} e^{-2\pi i q m} - 1 = (\dots) = \frac{\sin N\pi q}{\sin \pi q}.$$

For large N , this expression effectively becomes a sum of delta functions at points where q is integer. Applying this to all three dimensions, we get that $\mathbf{Q} = \mathbf{G}_{hkl}$, i.e.

$$\sum_{\mathbf{v}_{mnp}} = C \cdot \sum_{\mathbf{G}_{hkl}} \delta(\mathbf{Q} - \mathbf{G}_{hkl})$$

with some constant C , which can be determined by integrating both sides over the unit cell:

$$\int_{\text{cell}} d^3q \sum_{\mathbf{v}_{mnp}} = \int_{\text{cell}} d^3q C \cdot \sum_{\mathbf{G}_{hkl}} \delta(\mathbf{Q} - \mathbf{G}_{hkl}) = C.$$

To evaluate the left-hand side, we use

$$\int_{\text{cell}} d^3q e^{i\mathbf{q}(\mathbf{v}-\mathbf{v}')} = \frac{(2\pi)^3}{V_{UC}} \delta_{\mathbf{v}\mathbf{v}'}$$

and get

$$C = \frac{(2\pi)^3}{V_{UC}} \sum_{\mathbf{v}} \delta_{\mathbf{v}\mathbf{v}'} = \frac{(2\pi)^3}{V_{UC}}.$$

□

EXERCISE 6.2

Calculate the structure factor for a diamond lattice (an fcc lattice with a two-atomic basis at $(0, 0, 0)$ and $(a/4, a/4, a/4)$).

Solution. The atom positions for the diamond lattice are $(0, 0, 0)$, $(a/2, a/2, 0)$, $(a/2, 0, a/2)$, $(0, a/2, a/2)$, $(a/4, a/4, a/4)$, $(3a/4, 3a/4, a/4)$, $(3a/4, 0, 3a/4)$, $(0, 3a/4, 3a/4)$.

The structure factor is defined as (\mathbf{G}_{hkl} : reciprocal lattice vector, \mathbf{R}_j : position of atom j in the unit cell)

$$\begin{aligned} F_{hkl} &= \sum_j e^{-i\mathbf{G}_{hkl} \cdot \mathbf{R}_j} \\ &= e^{-i \cdot 0} + e^{-2\pi i(h+k)/2} + e^{-2\pi i(h+l)/2} + e^{-2\pi i(k+l)/2} \\ &= e^{-2\pi i(h+k+l)/4} + e^{-2\pi i(3h+3k+l)/4} + e^{-2\pi i(3h+k+3l)/4} + e^{-2\pi i(h+3k+3l)/4} \\ &= 1 + (-1)^{h+k} + (-1)^{h+l} + (-1)^{k+l} + (-i)^{h+k+l} + (-i)^{3h+3k+l} + (-i)^{3h+k+3l} + (-i)^{h+3k+3l} \\ &= \left[1 + (-1)^{h+k} + (-1)^{h+l} + (-1)^{k+l} \right] \left[1 + (-i)^{h+k+l} \right]. \end{aligned}$$

This is the fcc structure factor (4 for h, k, l all even or all odd, 0 else) modified by term that depends on $h + k + l$. The end result is:

$$F_{hkl} =$$

- 0 if h, k, l not all even or 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

□

EXERCISE 6.3

In a powder diffraction experiment with a material having a cubic unit cell and using a neutron wavelength of $\lambda = 1.5 \text{ \AA}$, the first few Bragg peaks occur at the scattering angles $\Theta = 43.31^\circ, 50.44^\circ, 74.12^\circ, 89.93^\circ$. Determine the structure (bcc, fcc, 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. The scattering angle is related to the lattice plane distance by the Bragg equation:

$$d_{hkl} = \frac{\lambda}{2} \sin \frac{\Theta}{2}.$$

The d_{hkl} for the given four angles are therefore $d_1 = 2.0323 \text{ \AA}$, $d_2 = 1.7600 \text{ \AA}$, $d_3 = 1.2445 \text{ \AA}$, and $d_4 = 1.0613 \text{ \AA}$.

Also, for a cubic unit cell, the plane distances are related to the lattice constant by

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

Now we need to look at the first four allowed reflexes of the simple cubic, bcc, and fcc lattices, assign them to the given d values. The structure is correct if we derive the same lattice constant a for all d values.

simple cubic: all hkl are allowed reflexes

reflex	d_{hkl}	a in Å	
100	a	2.0323	
110	$a/\sqrt{2}$	2.489	\Rightarrow no match!
111	$a/\sqrt{3}$	2.1555	
200	$a/2$	2.1226	

bcc: only allowed reflexes for $h + k + l$ even

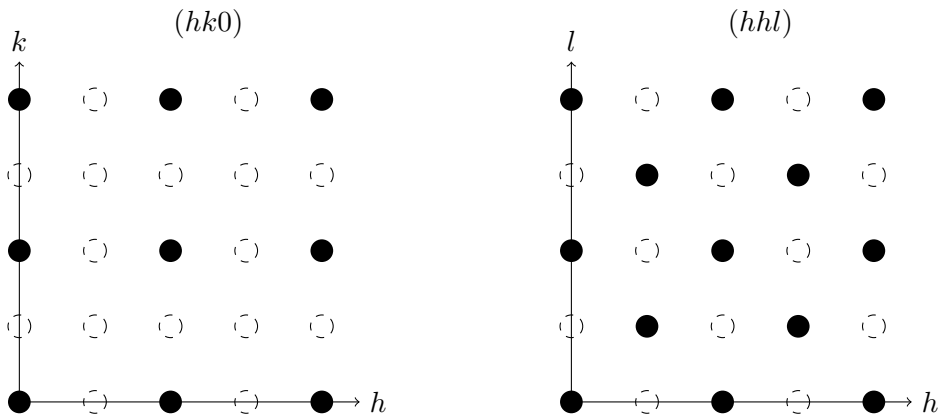
reflex	d_{hkl}	a in Å	
110	$a/\sqrt{2}$	2.874	
200	$a/2$	3.52	\Rightarrow no match!
211	$a/\sqrt{6}$	3.048	
220	$a/\sqrt{8}$		

fcc: only allowed reflexes for h, k, l all even or all odd

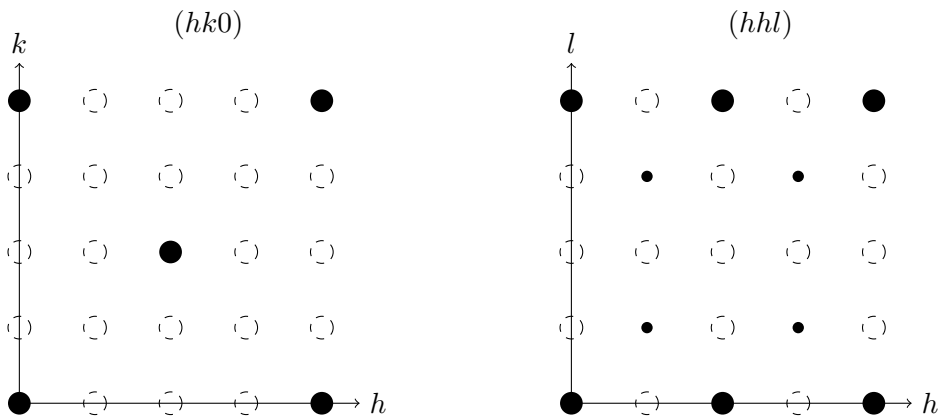
reflex	d_{hkl}	a in Å	
111	$a/\sqrt{3}$	3.52	
200	$a/2$	3.52	\Rightarrow match!
220	$a/\sqrt{8}$	3.5199	
311	$a/\sqrt{11}$	3.5199	

The structure is fcc with a lattice constant of $a = 3.52 \text{ \AA}$ (elemental Nickel).

FCC lattice planes with allowed reflexes:



Diamond lattice planes with allowed reflexes:



- = allowed
- = allowed, but weaker
- = forbidden

□

EXERCISE 6.4

1. Sample holders for diffraction experiments are often made of materials that do not scatter coherently (why?). A possible choice is a *zero-scattering alloy* which can be a mixture of natural titanium and zirconium. What is the composition of this alloy? Why is the term «zero-scattering» misleading?
2. A vanadium sample is a standard sample for calibration at many instruments. Can you think of a reason for that?

Solution. 1. In diffraction experiments, most of the time the interesting quantity is the coherent scattering of the sample (i. e. Bragg peaks). If the sample holder has Bragg peaks itself, subtraction is not so easy and more error-prone. To obtain an alloy that does not scatter coherently, the mean value of b of the components has to be zero:

$$c_{\text{Ti}} \cdot b_{\text{Ti}} + c_{\text{Zr}} \cdot b_{\text{Zr}} \stackrel{!}{=} 0$$

$$c_{\text{Ti}} \cdot (-3.438 \text{ fm}) + (1 - c_{\text{Ti}}) \cdot 7.16 \text{ fm} \stackrel{!}{=} 0$$

This is the case for $c_{\text{Ti}} = 68.6\%$ and correspondingly $c_{\text{Zr}} = 32.4\%$.

This alloy does not scatter coherently (if the occupancies of the sites is really statistically mixed), however it does scatter incoherently!

2. Vanadium is one of the few elements that scatter almost only incoherently (the cross sections are $\sigma_{\text{coh}} = 0.0184$ barn compared to $\sigma_{\text{inc}} = 5.08$ barn). Therefore, it scatters the same intensity in every solid angle element $d\Omega$. This measurement can therefore be used to calibrate the detector efficiency, shadowing effects, etc.

□