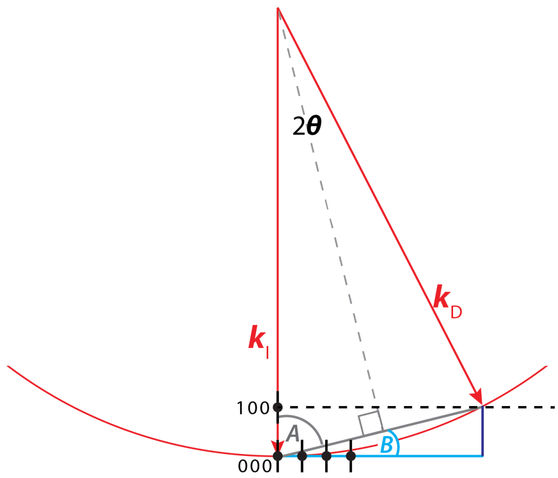
Assignment Week 4 – Answers

Assignment 4.1

a) The following diagram represents the problem to be solved, where 2θ is the TEM scattering angle for which the Ewald sphere cuts the first order Laue zone, which is represented by the black dashed line.



By labelling the length of the grey line as l, we can show:

$$l = 2\,|k_{\mathrm{I}}|\sin\theta \approx \frac{2\theta}{\lambda}$$

From trigonometry, angle $B = \theta$
Also, the length of the dark blue line corresponds to the reciprocal of $d_{1\,0\,0}$. Therefore:

$$\frac{1}{d_{1\,0\,0}} = l\sin\theta \approx l\theta$$

Combining with the above, we obtain:

$$\frac{1}{d_{1\,0\,0}} \approx \frac{2\theta^2}{\lambda} \Longrightarrow 2\theta \approx \sqrt{\frac{2\lambda}{d_{1\,0\,0}}}$$

For the 200 keV beam $\lambda = 2.51$ pm, and for a cubic material $d_{1\,0\,0} = a = 0.352$ nm. Therefore, the scattering angle at which the Ewald sphere crosses the first order Laue zone is:

$2\theta\ = 119$ mrad

b) Being a cubic system, the plane $(1\ k\ 1)$ has a plane spacing:

$$d_{1\,k\,1} = \frac{a}{\sqrt{1+k^2+1}} = \frac{a}{\sqrt{2+k^2}}$$

The length *l* corresponds to the reciprocal of this plane spacing. Therefore, using derivations from part (a):

$$l \approx \frac{\sqrt{2+k^2}}{a} = \sqrt{\frac{2}{\lambda a}} \Rightarrow k \approx \sqrt{2\left(\frac{a}{\lambda}-1\right)}$$

Substituting in values gives:

$k = 17$ (to the nearest whole number) and so the $(1\ k\ 1)$ FOLZ plane most likely to be excited is:

$(1\ 17\ 1)$

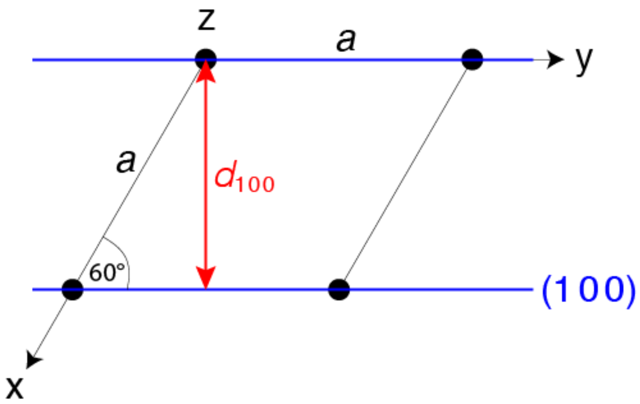
c) A reflection of the type $(1\ k\ 0)$ cannot be visible. This is because, for the FCC system, only planes with Miller indices h, k, l all even or all odd diffract. A plane $(1\ k\ 0)$ has mixed odd and even Miller indices, and so is a systematic absence.

Assignment 4.2

a) As can be seen on the schematic diagram below, showing a hexagonal unit cell in black and the $(1\ 0\ 0)$ lattice planes in blue, the perpendicular distance between $(1\ 0\ 0)$ lattice planes for a hexagonal unit cell, i.e. the lattice plane spacing, is given by:

$$d_{100} = a \cdot \sin 60° = a\frac{\sqrt{3}}{2}$$

For $a = 0.246$ nm, $d_{100} = 0.213$ nm



b) Taking the kinematical expression for I_g, the intensity in the diffracted beam:

$$I_g = I_0 \frac{\sin^2(\pi t s)}{(\pi t s)^2}$$

it can be seen that the first zero of intensity along the reciprocal lattice rod is when:

$$t = \frac{1}{s}$$

Also from the video lecture 4.3, we take the expression relating s to the tilting angle $\Delta\theta$:

$$s = \frac{\Delta\theta}{d_{hkl}}$$

Relating these two expressions, we obtain:

$$t = \frac{d_{hkl}}{\Delta\theta}$$

This $\Delta\theta$ is in rad, so for a value given in degrees $\Delta\theta(°)$ must be converted to rad:

$$t = \frac{d_{hkl}}{\Delta\theta(°)} \cdot \frac{180}{\pi}$$

Inserting the values $d_{100} = 0.213$ nm and $\Delta\theta(°) = 18°$ the following sample thickness is found:

$t = 0.68$ nm

Given this plane spacing and the tilting information, estimate the thickness of the bi-layer graphene sample. Note that the sample is sufficiently thin that the kinematical approximation for intensity distribution along the relrod is valid.

c) The thickness of the bilayer is a close match to the $c = 0.67$ nm lattice parameter of the graphite unit cell.

This is because the graphite unit cell contains two graphene layers in hexagonal lattice coordination, and the c lattice parameter corresponds to their combined thickness. That is, it corresponds to the thickness of a graphene bilayer.

d) As a first approximation, a single layer of graphene has zero thickness. Taking the Fourier transform of this will therefore produce infinitely long, uniformly intense relrods. As a result, the intensity measured in the diffraction spot will not vary as the sample is tilted and the reciprocal lattice cuts the uniformly intense relrods at different places.

(Note that this was essentially confirmed experimentally in the paper by Meyer et al., where only small intensity variations in the graphene diffraction spots were observed on sample tilting.)