PHY2009 Physics of Crystals:
Problems Sheet for lecture 10

1) Draw the lattice points (in real space) for a (001) plane for the hexagonal-P lattice. Calculate (or construct geometrically) the reciprocal lattice for this plane.

2) Using the Ewald Sphere Construction: For this exercise you ideally need a sheet of graph paper, an overhead transparency sheet (or tracing paper) and a compass. However, you should still get reasonable results using ordinary A4 paper, although you may need to hold the sheets up to the light to see through them!

   (a) Draw on the graph paper a square lattice of nearest-neighbour separation 3 cm. Using a scale of 1 cm = $2\pi/(1\text{ nm})$ this will be used to represent the reciprocal lattice of a square direct lattice of side 0.33 nm.

   (b) On the overhead transparency (or tracing paper) draw the Ewald sphere (= circle!) for incident radiation of wavelength 0.25 nm (if you only have one transparency, leave space for other circles for later on).

   (c) Show (using the Ewald Sphere Construction) that Bragg reflections having the two smallest Bragg angles, θ, occur at $\theta = 22^\circ$ and 32.5°, and write down the miller indices of the reflecting planes in each case (note: this is particularly easy using this construction – just identify the vector **G** involved and you are there!). How many Bragg reflections occur altogether, if the angle of the incoming wave (NB this is not the Bragg angle) is allowed to range from 0 to 90°, relative to a (10) direction of the lattice, but the reflected beam can be detected over the full 360°? [Answer: 10]

   (d) Confirm the two values for the Bragg angle obtained in (c), using the condition for diffraction: $k \sin\theta = G/2$.

   (e) Use the Ewald Sphere Construction to convince yourself that incident wavelengths less than 0.66 nm are required to see any Bragg reflections at all.

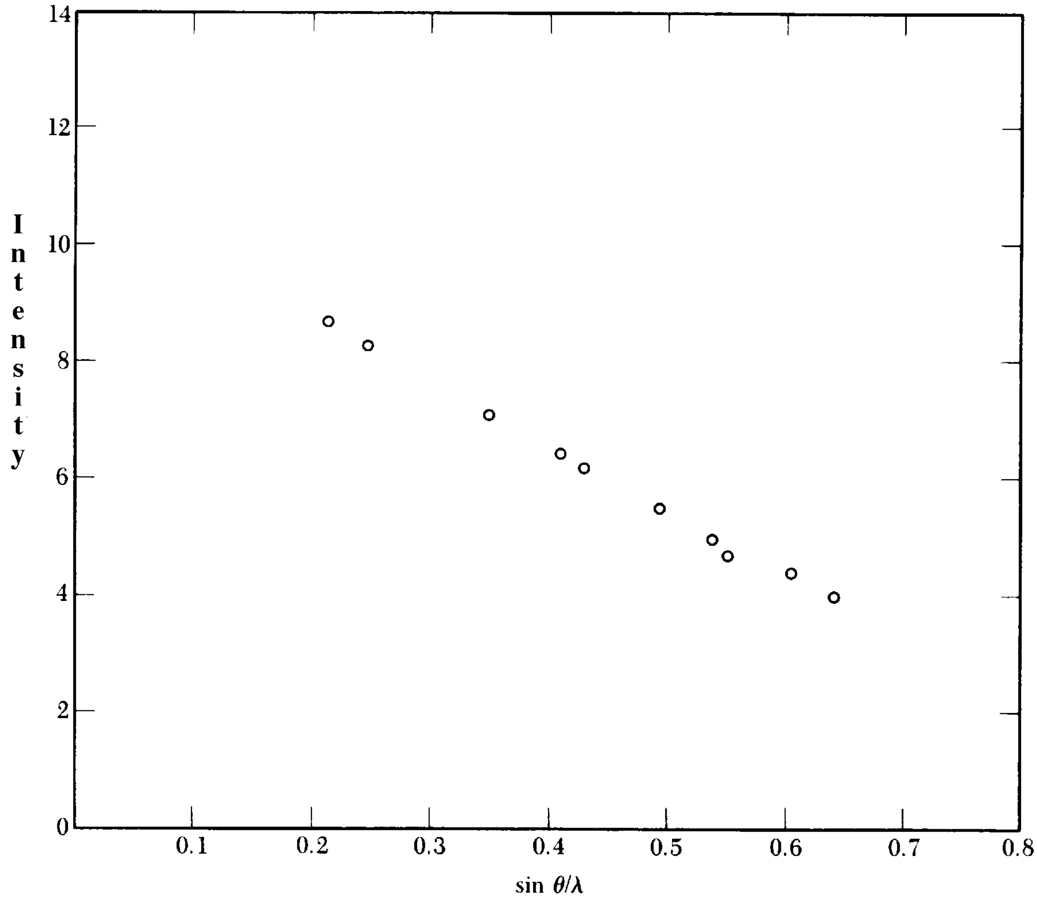
   (f) In a diffraction experiment using the Laue Method, the lattice above is illuminated with x-rays with wavelengths between 0.125 and 0.250 nm, which are incident along a (10) direction. Draw the Ewald Sphere construction for this experiment, and hence determine the number of reflections seen (assuming the experimental arrangement allows the observation of beams scattered in any direction). [Answer: 17]

Rob Hicken, November 2004

PHY2009 Physics of Crystals:

Supplementary Problems on Scattering

1) The figure shows the Bragg angles for the diffraction peaks observed when x-rays scatter off aluminium powder, which is known to crystallise in one of the cubic lattice types. The units of the horizontal axis are $Å^{-1}$.



(a) Write down the conditions on the Miller indices $(hk\ell)$ for allowed Bragg reflections for the three cubic lattice types.

(b) By considering the ratios of the sines of the Bragg angles in the figure, determine the Bravais lattice of aluminium.

(c) Hence label each of the Bragg peaks shown with its Miller indices.

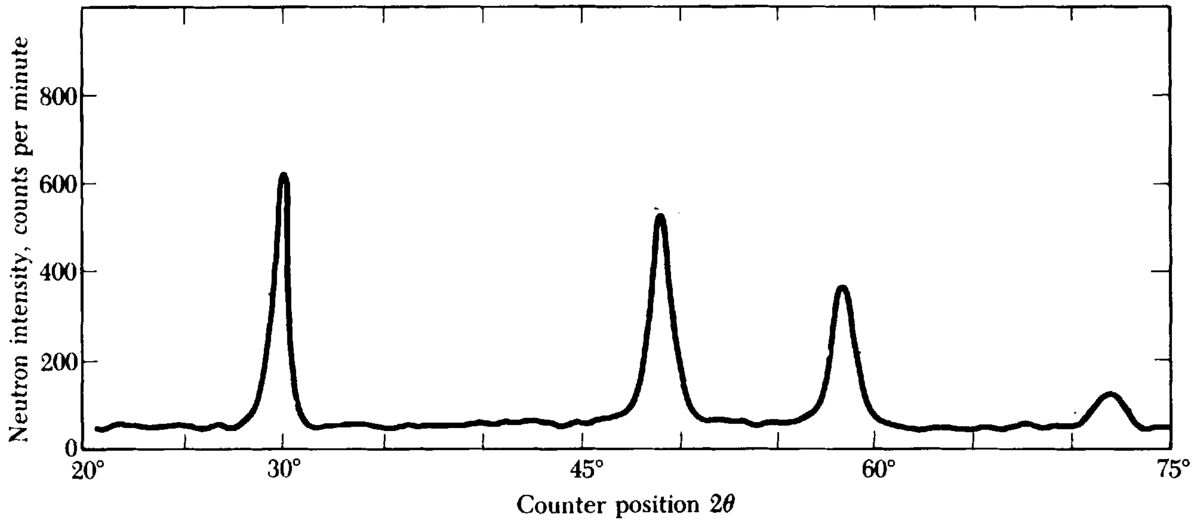
(d) Given that molybdenum Kα x-rays (λ = 0.713 Å) were used in this experiment, calculate the conventional cubic lattice constant of aluminium. [answer: 4.05 Å]

Rob Hicken, Novmeber 2004

2) The Bragg angle for a certain reflection from a powder specimen of copper is 47.75° at a temperature of 293 K and 46.60° at 1273 K. Calculate the coefficient of linear thermal expansion of copper. [answer: 1.91×10^{-5} K^{-1}]

[Hint: a quick method involves differentiating the Bragg condition – if you use this method, you must express your angles in radians.]

3) The figure shows the scattering angles for Bragg reflections observed in a neutron diffraction experiment carried out on a powdered sample, which is believed to have a simple cubic, body-centred cubic, face-centred cubic or diamond structure.



(a) Write down the conditions on the Miller indices $(hk\ell)$ for Bragg reflections to be observed for each of the candidate structures.

(b) Use the data in the figure to determine the crystal structure of the powder.

(c) Label each peak with its Miller indices.