020221 Quiz 6 XRD

1) **Why** does the Lorentz function, $(1 + \cos^2 2\theta)$ depend on 2θ rather than θ?
   What is the origin of the two terms in this expression?
   Would this expression work in this form for synchrotron radiation (polarized x-rays)?

2) **At what range** of 2θ would you measure the Compton background which needs to be subtracted from diffraction patterns when using the intensity?
   Explain why this range would be selected.

3) **Sketch** the general form of the atomic scattering factor, f.
   Why does this factor take this shape?
   What is the value at the $2\theta \Rightarrow 0$ intercept?

4) **Calculate** the structure factor, $F^2_{hkl}(2\theta)$, for a FCC crystal (be sure to include f). Do this by:
   Listing the atom positions in the unit cell
   Calculating the phase for each atom
   Summing terms in the expression for the relative amplitude of a scattered wave
   Squaring the amplitude to obtain $F^2_{hkl}(2\theta)$
   Give general rules for FCC based on the hkl values.
   Make sure your expression predicts known features such as the absence of a 100 peak.

Answers: 020221 Quiz 6 XRD

1) The Lorentz function, $(1 + \cos^2 2\theta)$ depends on 2θ rather than θ because it relates to the angle between the E field vector and the direction of the scattered wave. This angle $\alpha = 90-2\theta$ so $\sin^2\alpha = \cos^2 2\theta$, for in-plane scattering and 1 for out of plane scattering since α is always 90 for this condition. The mean of these two terms gives the Lorentz expression for unpolarized x-rays. The expression would not work in this form for synchrotron radiation which is polarized. You would need to know the direction of detection relative to the direction of polarization to determine the correct expression at a synchrotron.

2) The Compton background is measured at high angles since high angles relates to large wavelength by Bragg's law and large wavelength relates to low frequency, where incoherent inelastic effects reach a maximum.

3) f decays from Z to 0 and has a knee/leg shape as seen in the notes. It takes this shape because of electron/electron correlation within the atomic orbitals at small sizes or high angle. The value at 0 angle is Z, the number of electrons in the atom.

4) This is done in the notes.