Quiz 7 XRD

The diffracted intensity can be calculated for a diffractometer with unpolarized x-rays by the following equation:

$$I(2\theta) = K\left|F^2\right| p\left(\frac{1+\cos^2 2\theta}{\sin^2\theta\cos\theta}\right) e^{-\left(q^2\sigma^2\right)/2}$$

where K is a constant proportional to $1/R^2$.

a) **How** would "p" be different for (110) and (111) reflections (you can count the normals to the planes if it helps).

b) **Explain** why a (110) reflection is not observed for an FCC structure.
Explain which term determines what reflections are not observed.
Calculate this term using complex numbers generally for an FCC structure and for this plane.
Give a general rule that applies to whether reflections are observed for FCC structures.

c) The term containing trigonometric functions is calculated in two parts that pertain to the numerator and the denominator.
Explain the origin of the numerator (top).
A crystal monochromator partially polarizes x-rays in the plane of reflection.
Will this effect this term if the monochromator is before the sample?
What about if it is after the sample?

d) **Give** a general description of the source of the denominator in the term containing trigonometric functions.
Would this term vary for a flat film detector such as the Polaroid film used in some of the labs? **Explain**.

e) **What** is σ in the last term?
What is the source of this term?
Describe the effect of this term as a function of 2θ?

Answers: Quiz 7 XRD

a) Normals to the (110)'s are the edges and normals to the (111)'s are the corners. There are 8 corners and 12 edges on a cubic unit cell so the ratio of p's for (110) and (111) is 1.5.

b) This is derermined by $|F^2|$.

FCC has 4 atoms at [000], [1/2,1/2,0], [1/2,0,1/2], [0,1/2,1/2] so,

$F = f\,(1 + e^{-i\pi(h+k)} + e^{-i\pi(h+l)} + e^{-i\pi(k+l)})$

For the (110) plane this is

$F = f\,(1 - 1 - 1 + 1) = 0$

Mixed hkl $|F^2| = 0$; unmixed hkl, $|F^2| = 4\,f^2$.

c) The numerator is from the Thompson equation for scattering from a single electron. This depends on the angle between the electric field vector of the incident beam and the direction of propagation of the scattered beam, $I(2\theta) = K \sin^2\alpha$. If **E** is in the plane of detection $\sin^2\alpha = \cos^2 2\theta$. If **E** is normal to the plane of detection $\sin^2\alpha = 1$. The numerator is an average of these two cases for unpolarized radiation.

If the monochromator is before the sample the term is either $\cos^2 2\theta$ or 1 depending on the direction of polarization. If the monochromator is after the sample, the Thompson effect is not altered but the diffracted beam is partially polarized and the monochromator should be normal to the plane of detection for maximum detected intensity.

d) The denominator arises from geometric effects in the diffractometer as described in Stock and Cullity or in the web notes.

The term would vary depending on the geometry of the detection.

e) σ is the root mean square (rms) motion of atoms due to thermal vibrations. σ^2 is proportional to kT.

This function describes an exponential decay in $\sin^2\theta$, so a decay in 2θ. The intensity will generally decay with angle due to thermal vibrations.