XRD Homework 5

1.) a.) In class we discussed the diffraction pattern for a mono-atomic ideal gas. How is this related to the atomic form factor used to calculate the diffraction intensity?

b.) Explain how a collection of these diffuse patterns can lead to the sharp peaks of an XRD pattern from a crystal.

c.) For an amorphous solid or a liquid there is a broad "halo" in the XRD pattern. What causes this?

d.) Why do closest packing diffraction peaks appear to grow out of this amorphous halo on crystallization?

e.) The atomic form factor, f, is a scattering amplitude function rather than an intensity function. Why is f used to calculate the diffracted intensity rather than f^2 (f^2 is directly related to the scattered intensity)?

2.) The Ewald Construction for the powder method (fig. A1-11, pp. 492) consists of two spheres depicted as circles in a 2-d plot.

a.) How are the incident and diffracted beams represented in this construction?

b.) Where is the origin of reciprocal space in this construction?

c.) What is the relationship between the cone of reflection seen in figure A1-10 and a Debye-Scherrer ring observed in the diffraction pattern.

d.) In terms of the reciprocal lattice, why are all possible reflections with d-

spacings larger than /2 observed in a powder pattern (i.e. what manipulations of the reciprocal lattice are necessary to obtain all of these reflections)?

e.) In terms of the reciprocal lattice, what is the origin of the /2 limit to Bragg's Law?

3.) a.) Explain why a diffracted wave is out of phase with the incident wave by /2.b.) Why doesn't this have an effect on the calculation of the diffracted intensity?

c.) What effect will this have at 2 = 0?

d.) X-rays from a synchrotron are polarized (also x-rays which pass through a Soller slit can be partially polarized). What effect will this have on equation 4-2 pp. 110? You will need to assume a direction of polarization for this problem.