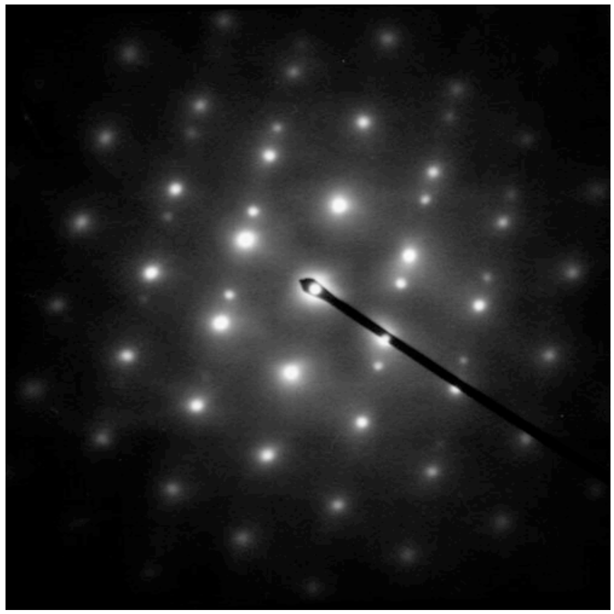
090522 Quiz 5 XRD

1) Construct the Sphere of Reflection by sketching a reciprocal lattice with an origin, (000) and the center of the diffraction measurement indicating 2θ and $(\mathbf{S} - \mathbf{S_0})/\lambda$. Why are only a few peaks seen when a perfect crystal diffracts with a single wavelength x-ray radiation?

2) The following electron diffraction pattern is from an austenite phase of steel. Explain how this relates to inverse space and why electron diffraction patterns appear different than x-ray diffraction patterns.



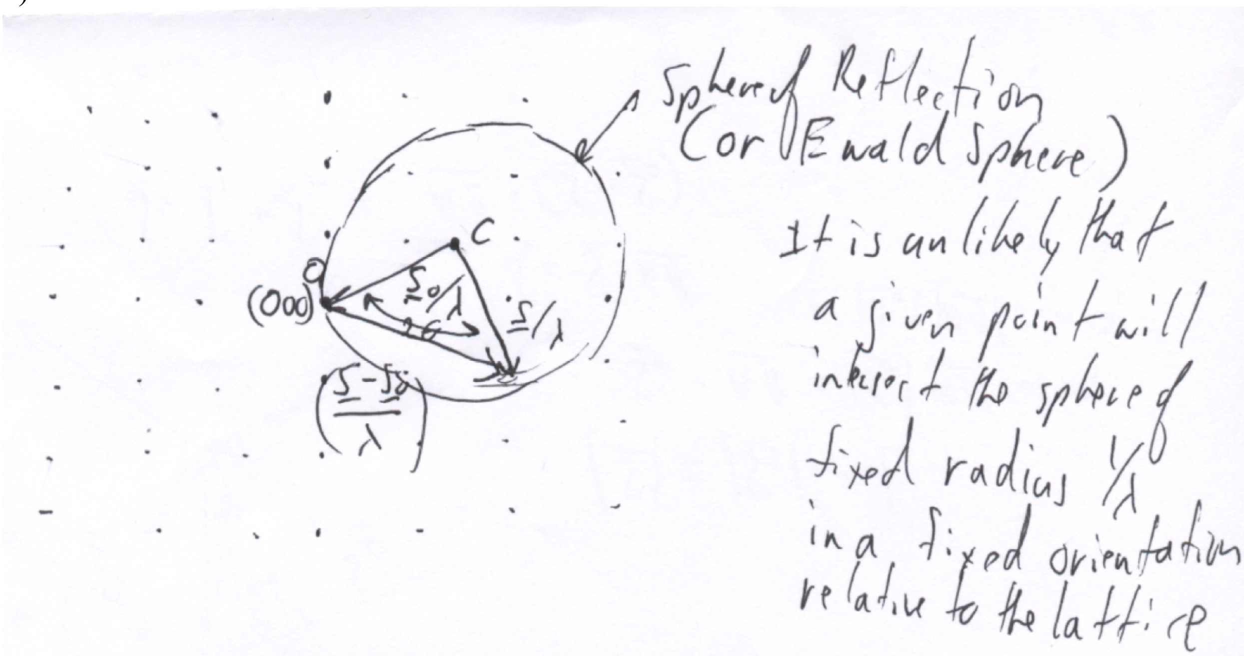
3) Construct the limiting sphere and explain why Debye-Scherrer rings are seen from a powder pattern in a 2D photographic measurement such as was done in lab 2.

4) Explain why for FCC the unit cell structure factor, F, is 4f for unmixed hkl and is 0 for mixed hkl where f is the atomic form factor.

5) Sketch the atomic form factor (I versus 2θ) and explain why the function has this shape.

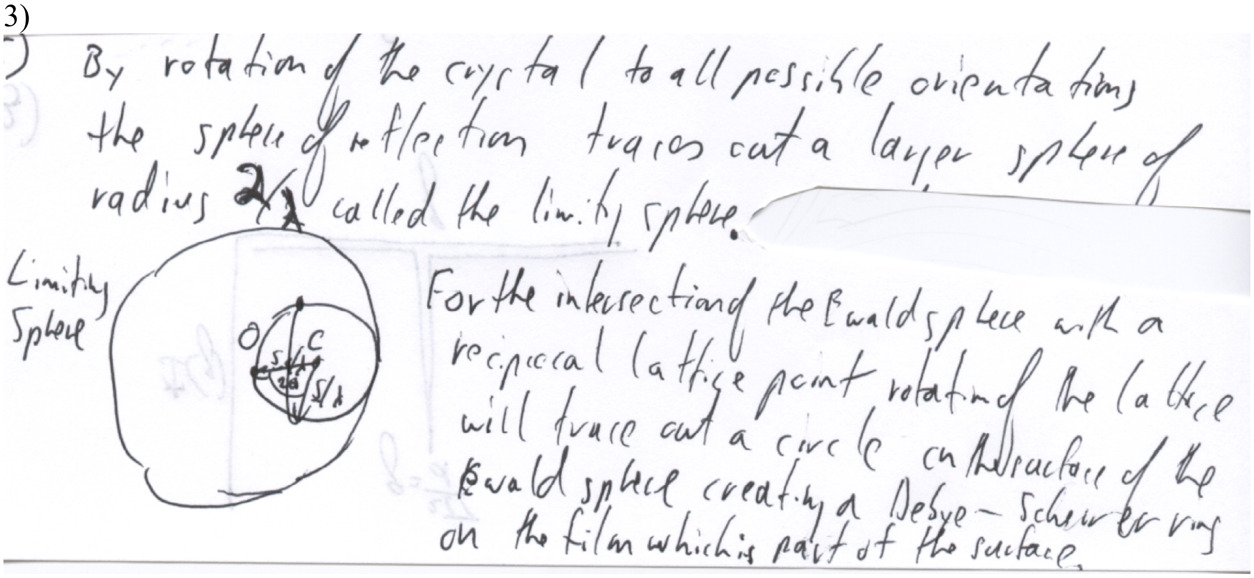
Answers: 090522 Quiz 5 XRD

1)



2) The wavelength of electrons is two orders smaller than the wavelength of x-rays so the sphere of reflection is two orders larger in diameter. The sphere is basically close to a flat sheet compared to the lattice size so we observe many more reflections in the electron diffraction pattern compared to an x-ray diffraction pattern. The Ewald sphere for electrons can align with the inverse space lattice to yield many reflections as shown in the figure.

3)



4) 4 atoms (0,0,0); (1/2,1/2,0); (1/2,0,1/2); (0,1/2,1/2)

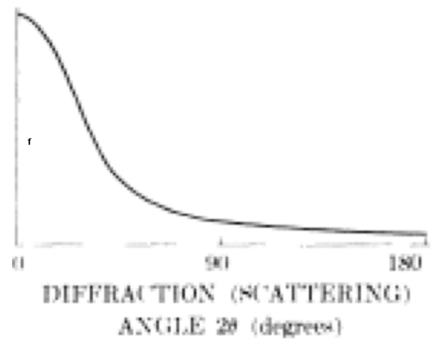
$$F = f[1 + e^{(\pi i(h+k))} + e^{\pi i(h+l)} + e^{\pi i(k+l)}]$$

for Unmixed hkl => $F = 4f$ and $F^2 = 16f^2$

for Mixed hkl => F = 0

i.e. no (100) reflections but will have (111), (200) etc.

5) Plot of f versus 2 θ.



f shows a monotonic decay with 2 θ because it represents the Fourier transform of the electron density distribution function for an electron cloud which is basically a Gaussian (bell shaped) function. The Fourier transform of a Gaussian is another Gaussian which is a monotonic decay curve of the type shown above.