061025 Quiz 5 XRD

1 & 2) It was mentioned in Lab 1 that the diffraction pattern observed on a film or screen is the Fourier transform of the structure. Explain how a diffraction pattern with one peak (one d-spacing) is related to the real space structure of a crystal using the pairwise correlation function (rod throwing probability) and a Fourier transform of this function.

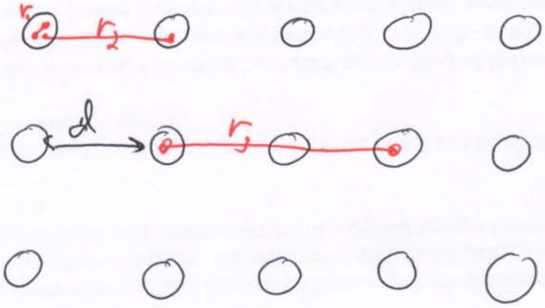
3) Show how the phase difference, $\phi = 2\pi/\lambda\ (\mathbf{S} - \mathbf{S_0}) \bullet \mathbf{AB}$ can be obtained from a sketch of the diffraction from atoms A and B.

4) 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?

5) 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.

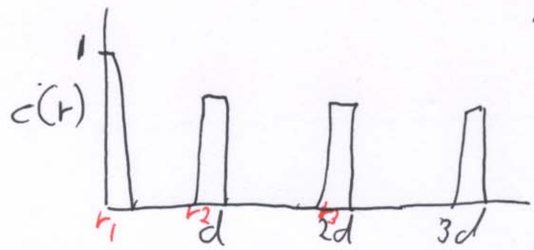
ANSWERS 061025 Quiz 5 XRD

1)

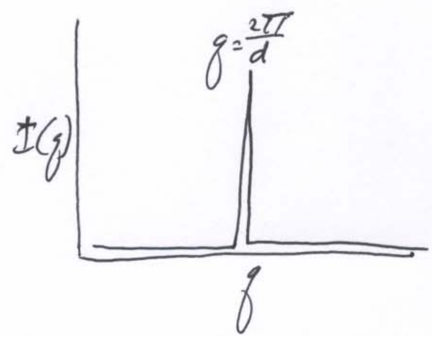


Consider only one d-spacing

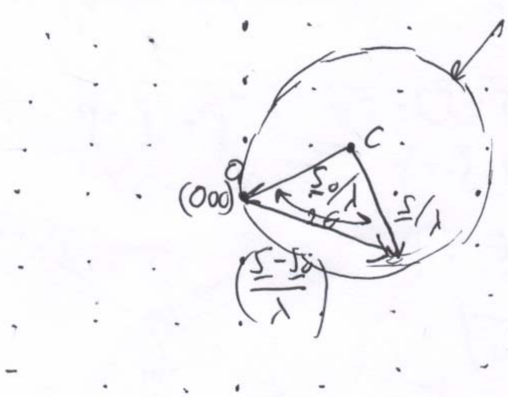
1) Probability of a rod in phase of the atoms is one at $r=0$ then 0 at $r >$ the atom size but $r < d$ and high at $r = d$ etc.



This correlation function can be represented by a single sin wave of wavelength d
So the resulting FT is single valued

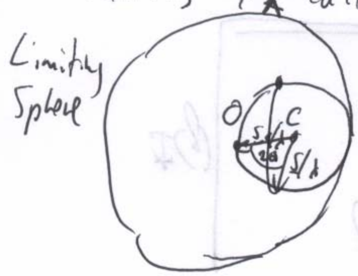


4)



It is unlikely that a given point will intersect the sphere of fixed radius $1/\lambda$ in a fixed orientation relative to the lattice

5) By rotation of the crystal to all possible orientations the sphere of reflection traces out a larger sphere of radius $2/\lambda$ called the limiting sphere.



For the intersection of the Ewald sphere with a reciprocal lattice point rotation of the lattice will trace out a circle on the surface of the Ewald sphere creating a Debye–Scherrer ring on the film which is part of the surface.