Quiz 5 4/27/01 XRD

a) **Derive** Bragg's Law for two atomic planes using the specular analogy.
Indicate what part of your derivation relies on the specular assumption.

b) **Show** how the Scherrer equation can be obtained from an incremental derivative of Bragg's Law.

c) If you identify a diffraction peak as a (100) reflection from a cubic crystal:
What information can you obtain from a diffractometer trace (I versus 2θ) of the peak given the peak has a fairly large breadth and the intensity is in absolute units?
What other information can be obtained from a 2-d detector such as the Polaroid film?

d) **Sketch** reciprocal space for a diffraction measurement as done in class including $\mathbf{S}_0/\lambda$, $\mathbf{S}/\lambda$ and a simple cubic lattice making sure to indicate the origin of the reciprocal lattice and the center of the diffraction experiment.
How can the creation of a diffraction peak be described in this sketch?
What decides the orientation of $\mathbf{S}_0/\lambda$ relative to the reciprocal lattice?

e) **What** is the limiting sphere?
What is limited by the limiting sphere?

Answers: Quiz 5 4/27/01 XRD

a) The specular assumption is that the incident angle must equal the diffraction angle. Derivation is in the notes.

b) This is the Sathish derivation from the notes.

c) You can determine at least three things from the diffractometer trace, the composition, the d-spacing and the crystal size. The polaroid film allows a determination of the crystal orientation.

d) Sketch is in notes.
A diffraction peak occurs when the sphere of reflection intersects a reciprocal lattice point.
The orientation of $\mathbf{S}_0/\lambda$ relative to the reciprocal lattice is decided by the sample orientation in the diffractometer.

e) The limiting sphere is obtained by spinning the sphere of reflection about the origin for all angles. This describes the limit of reciprocal lattice points that can possible give rise to a diffraction peak for the wavelength you are using.