020214 Quiz 5 XRD

1) -Show how the Scherrer equation can be obtained from Bragg's Law.
   -What else could lead to line broadening in XRD (observed in aluminum for instance).
   -Give an equation that describes such broadening in the diffraction pattern of aluminum at high temperature.

2) -Sketch the diffraction experiment in reciprocal space showing:
   -the vectors $\mathbf{S}/\lambda$ and $\mathbf{S}_0/\lambda$,
   -the origin of reciprocal space (000),
   -the center, C, of the measurement,
   -a typical reciprocal lattice,
   -the angle 2θ,
   -the sphere of reflection
   -and the limiting sphere.
   -How does this construction relate to the diffractometer trace of I versus **q** (reduced 2θ, $|\mathbf{q}| = 4\pi/\lambda \sin(\theta)$)?
   -How is the orientation of the crystal with respect to the incident x-ray beam described in this sketch?

3) Describe the Laue measurement using reciprocal space.
   -Sketch a transmission Laue pattern and explain how it is formed using reciprocal space.
   -Sketch a back-reflection Laue pattern (measured in lab) and explain how it is formed using reciprocal space.

Answers: 020214 Quiz 5 XRD

1) -See notes: Sathish Sukumaran's derivation Chapter 3.
   -Debye thermal broadening which is caused by thermal motion of the atoms in a crystal.
   -The diffraction peak is described by a Gaussian function (bell shaped curve) in q,
   $I(q) = I_{peak} \exp(-(q-q_0)^2\sigma^2)$, where q is $4\pi/\lambda \sin(\theta)$ and q_0 is the position of the peak. s is the mean free path of the atom at the lattice position.

2) -See notes: reciprocal road map and book, appendix 1.
   -q is a reciprocal space vector that is proportional to $\mathbf{S} - \mathbf{S}_0$. This vector goes from (000) to the surface of the sphere of reflection. The diffractometer trace reflects a line from (000) along the surface of the sphere of reflection and "I" indicates intersection of the reciprocal lattice with the sphere of reflection.
   -The angles describing the intersection of $\mathbf{S}_0$ with the reciprocal lattice at (000) describe the orientation of the crystal with respect to the incident x-ray beam.
3) -A zone axis (vector) in real space is represented as a plane in reciprocal space that passes through (000). Reciprocal lattice points lying on this plane make up the arcs seen in a Laue pattern. For forward scattering ellipses that pass through the main beam (000) are formed by intersection of the zone axis plane with the sphere of reflection. The center of this ellipse reflects the normal to the plane in reciprocal space which is the direction of the zone axis in real space. For back-reflection the plane (zone axis) intersects the sphere of reflection in hyperbolas that do not intersect the center of the pattern. The zone axis (normal to the plane) is not seen on the back-reflection pattern.