041021 XRD Quiz 4

Bragg's Law can be derived by considering the geometry of a reflected beam of electromagnetic radiation, the so called "specular analogy".

a) In what way does diffraction differ from reflection? (I can think of 3 major ways there may be more.)

b) Derive Bragg's Law using the reflection analogy.

c) Bragg's law is used to describe the relationship between the diffraction angle, and the d-spacing for a fixed wavelength radiation. The breadth of the diffraction peak is often related to the nano-crystallite grain size using the Scherrer equation. Show how the Scherrer equation can be obtained from Bragg's law using a derivative.

d) A crystal can display some degree of disorder and the disorder can take several distinct forms. Disorder of the first kind is associated with a gradual failure of the crystal unit cell to repeat in space in a given direction. If you used the Scherrer equation for large grain crystals ($>>10$ μm) that exhibited residual stress (which causes lattice distortions of the first kind), what would the Scherrer thickness, "t", correspond to?

e) Another type of disorder is random misplacement of atoms about their lattice location while maintaining coherence of the lattice over very long distances, disorder of the second kind. This might be associated with thermal vibrations in aluminum for instance. If you used the Scherrer equation to measure "t" for such a system (large grains, $t>>>10$μm, with disorder of the second kind) what would t correspond to? *(To answer this you might think about a native size scale that is manifested in thermal motion about a lattice site.)*

ANSWERS: 041021 XRD Quiz 4

a) The angle of incidence, θ, is defined by "d" for diffraction (interference) while it is free for reflection. Diffraction occurs only when multiple planes are correlated while reflection occurs for a single isolated surface. Diffraction requires a fixed wavelength (monochromatic radiation) to produce constructive interference while reflection is independent of wavelength.

b) see web notes for derivation.

c) see web notes for derivation.

d) The Scherrer thickness for disorder of the first kind reflects a coherence length for the crystal repeat. That is the distance beyond which the crystal does not repeat exactly the lattice in space.

e) For disorder of the second kind the Scherrer thickness would reflect the root mean square (RMS) distance of motion of the atoms at a lattice site, $<\sigma^2>^{1/2}$. This is the average diameter over which the atom moves or is displaced to a probability of 1/e. That is the fraction of atoms displaced to a distance σ or less is 1/e. Usually the Debye-Waller function is used to describe such Brownian motion about a lattice site,

$$I(q) = I_0 \exp(-(q-q_0)^2\sigma^2)$$

where I_0 is the intensity at the peak value for the diffraction peak, q is $4\pi/\lambda \sin \theta$, the magnitude of the inverse space vector, q_0 is the peak value of q from Bragg's law and σ is related to the RMS distance of motion. (Debye used σ to calculate the heat capacity of metals from diffraction data in work that was later awarded the Nobel prize.)

The exponential function, above, is sometimes called "a Gaussian" function since it was originally used by Gauss to describe a random system. Its form is that of a bell shaped curve so it is used for grade distributions to obtain the mean and standard deviation replacing q with the grade value and I with the number fraction of students. The standard deviation is proportional to σ and the mean is q_0. The Gaussian function is probably the most important function in science/engineering since it allows us to quantify disorder in nature.