090511 XRD Quiz 4

1) Derive Bragg's law assuming mirror-like behavior (specular analogy). Show all steps. How is diffraction similar to and how is it different from reflection?

2) Sketch the diffraction pattern from a crystal, amorphous or liquid, and from an ideal gas. Explain the differences, e.g. what is the structural difference between a liquid and a gas, and between a liquid and a crystal.

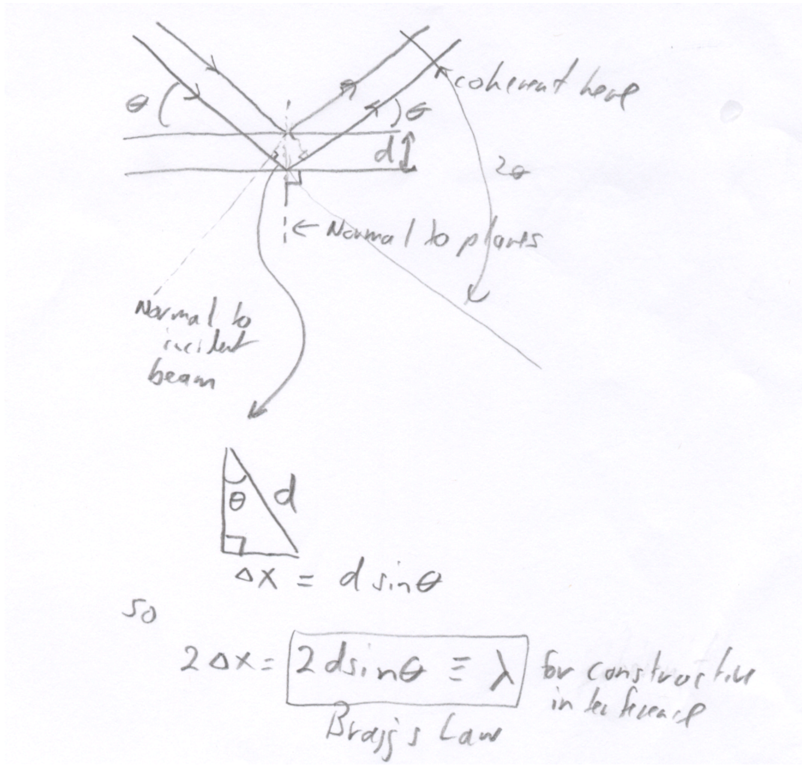
3) How do the Miller indices and inverse space unit vectors $\mathbf{b}_1$, $\mathbf{b}_2$ and $\mathbf{b}_3$ relate to the momentum analysis of diffraction (from Quiz 1)?

4) Give several examples (Cu, Al, Au, Zn etc.) of BCC, FCC and HCP crystal structures, the StructurBericht symbol for each structure, and the number of atoms per unit cell.

5) Derive the Scherer equation using a derivative of Bragg's Law. What is measured using the Scherer equation?

ANSWERS 090511 XRD Quiz 4

1)



Diffraction follows the angular rules of reflection in that the incident angle is equal to the exiting angle (the specular analogy). It is different from reflection in that for only one d-spacing will diffraction be observed at a given angle. Reflection occurs for any angle.

2)

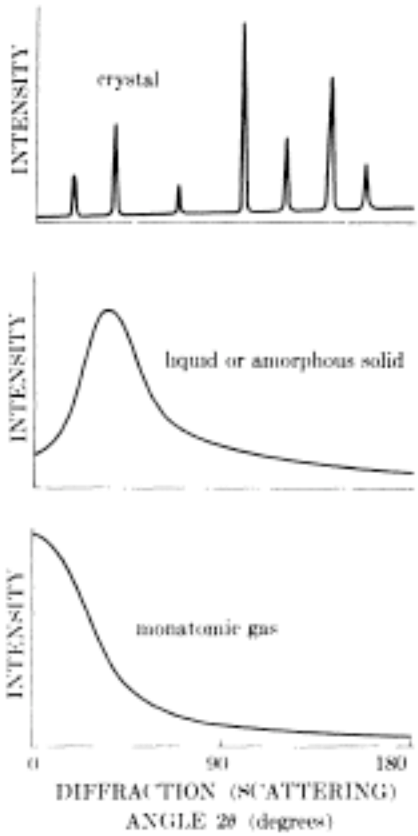
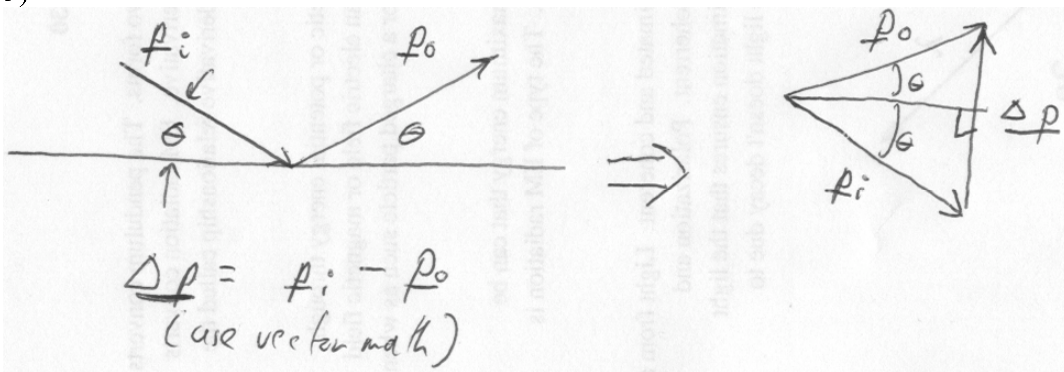


Fig. 3-18. Comparative x-ray scattering by crystalline solids, amorphous solids, liquids, and monatomic gases (schematic).

Cullity: "This relation between destructive interference and structural periodicity can be further illustrated by a comparison of x-ray scattering by solids, liquids, and gases (Fig. 3-18). The curve of scattered intensity vs. 26 for a crystalline solid is almost zero everywhere except at certain angles where high sharp maxima occur: these are the diffracted beams. Both amorphous solids and liquids have structures characterized by an almost complete lack of periodicity and a tendency to "order" only in the sense that the atoms are fairly tightly packed together and show a statistical preference for a particular interatomic distance; the result is an x-ray scattering curve showing nothing more than one or two broad maxima. Finally, there are the monatomic gases, which have no structural periodicity whatever; in such gases, the atoms are arranged perfectly at random and their relative positions change constantly with time. The corresponding scattering curve shows no maxima, merely a regular decrease of intensity with increase in scattering angle."

3)



Δp is normal to the plane. It has a magnitude of $\left|\underline{\Delta p}\right| = \frac{2h}{\lambda}\sin\theta = \frac{h}{d}$ so it is inversely related to distance or d-spacing. The vector h $\mathbf{b}_1$ + k $\mathbf{b}_2$ + l $\mathbf{b}_3$ is normal to the plane hkl and has a magnitude that is inverse to the plane spacing in units of the unit cell dimension a for a cubic lattice. When the inverse space vector equals the momentum change vector we observe diffraction.

4) Copper FCC 4; Aluminum FCC 4 **A1**; Zinc HCP 6 **A3** or 2; Magnesium HCP 6 **A3** or 2.
α-iron BCC 2 **A2** (others Li (at room temp.), Na, K, V, Cr, Fe, Rb, Nb, Mo, Cs, Ba, Eu, Ta); γ-iron FCC 4 **A1**; Silicon FCC (diamond type **A4**) 8; diamond FCC 8 **A4**
NaCl FCC 8 **B1**; KBr FCC 8 (NaCl type **B1**); Lead FCC 4 **A1**; Nickel FCC 4 **A1**.

5) The Scherer equation measures the size of a crystal grain if the grain is on the nanometer scale in size.

Sathish Sukumaran's Derivation of Scherrer Equation (010220)

Bragg's law is given by,

$\lambda = 2d\sin\theta$ (1)

Multiply both sides by an integer m such that md=t, the thickness of the crystal. This leads to,

$m\lambda = 2md\sin\theta = 2t\sin\theta$ (2)

Eqn. (2) can also be interpreted as the mth order reflection from a set of planes with a interplanar distance t.

Differentiate both sides of eqn. (2) remembering ml is a constant. This gives,

$0 = 2\Delta t\sin\theta + 2t\cos\theta\Delta\theta$ (3)

Remembering that as D q can be positive or negative (we are only interested in absolute values) leads to,

$t = \frac{\Delta t\sin\theta}{\cos\theta\Delta\theta}$ (4)

Since the smallest increment in t is d, using D t=d, and substituting l /2 for dsinq (from Bragg's law) we get,

$t = \frac{\lambda}{2\cos\theta\Delta\theta}$ (4)

Substituting B for 2D q , the angular width, we get,

$t = \frac{\lambda}{B\cos\theta}$ (5)

which is essentially Scherrer equation.

A more sophisticated analysis of the problem only adds a prefactor of 0.9 to the right hand side of eqn. (5) and leads to the correct Scherrer equation.

$t = \frac{0.9\lambda}{B\cos\theta}$ (6)