041029 Quiz 5 XRD

There is a 1 to 1 relationship between the structure of a material in real space (the crystal lattice or the density probability function discussed in class) and the structural observation in reciprocal space (the diffraction pattern).

a) Consider a vector of variable length "r" in real space and a powder pattern diffractometer trace. Plot the average probability, p(r), of finding atoms as a function of distance, "r", from a given atom for a crystal, a liquid (or glass) and an ideal gas (or an isolated atom).

b) In the context of the plot you have made for a liquid, what is the correlation hole (or excluded volume)?

c) Sketch the scattered (diffracted) intensity, $I(2\theta)$, as a function of scattering angle, 2θ, for a crystal (powder pattern), a liquid, and for an ideal gas (atomic form factor).

d) How does the correlation hole of part "b" manifest itself in the liquid diffraction (scattering) pattern of part "c"?

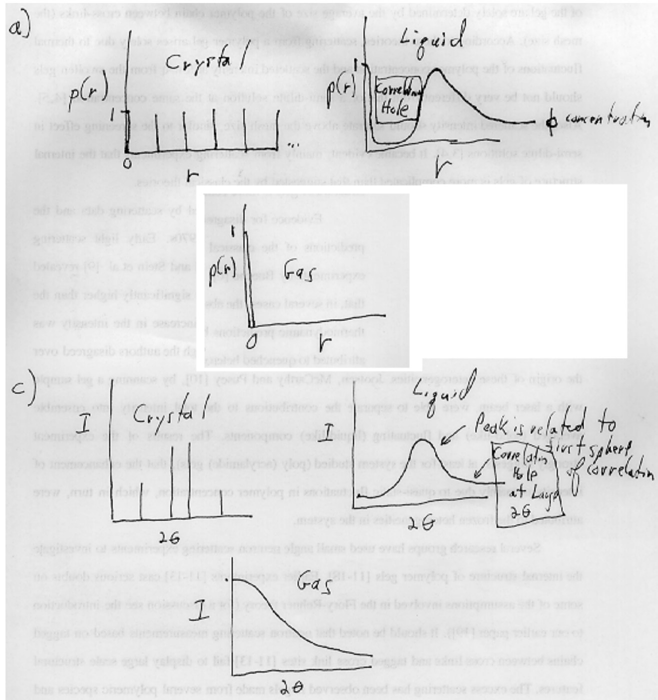
e) The condition for diffraction is met when the scattering vector '**s**' ends on a point in the reciprocal space. This can be given by the relationship,

$$\mathbf{s} = (\mathbf{S} - \mathbf{S_0})/\lambda = h\mathbf{b_1} + k\mathbf{b_2} + l\mathbf{b_3} = \mathbf{H}$$

where $\mathbf{S}$, and $\mathbf{S_0}$ are vectors in the scattered and incident directions, and $\mathbf{H}$ is a point in the reciprocal lattice. Derive the three Laue equations from the above equation.

ANSWERS: 041029 Quiz 5 XRD

a)



b) Correlation hole is the low "r" plateau caused the exclusion of other atoms from an atom that occupies volume.

d) Correlation hole corresponds directly with the high angle drop in intensity but is also associated with the diffuse peak in intensity.

e)
$$a_1 \bullet (S - S_0) = \{(a_1) \bullet (hb_1 + kb_2 + lb_3)\}\lambda = h\lambda$$

Similarly the dot products of a2 and a3 with the scattering vector give the remaining two Laue equations.