Quiz 6 XRD 5/4/01

X-rays display both a wave and a particle nature. This has implications for our understanding of the diffraction measurement.

a) The wave nature involves considering the phase difference between waves that are emitted from different atoms in the crystal.
Write an expression for the phase of an x-ray, φ, that arises from an atom at position [uvw] in a crystal and is contributing to a diffraction peak related to planes (hkl).
Explain how this expression can be obtained from the dot product of a real space and a reciprocal space vector (just show how the dot product works out).

b) **Explain** how this expression relates the observed diffraction angle with the crystal structure and the atoms giving rise to a diffraction peak.

c) Consider the particle nature of an x-ray. In this view the diffraction event involves an elastic collision of a photon with a tightly bound electron (doesn't move).
Write an expression for the momentum of a photon and
Show that the change in momentum on elastic scattering is related to $(\mathbf{S} - \mathbf{S}_0)/\lambda$ from the reciprocal space analysis. (Make a sketch of the diffraction measurement using photons and calcualte the momentum change.)
How is $\mathbf{q} = 4\pi \sin\theta/\lambda = 2\pi/d$ related to the change in momentum you calculated?

d) Explain that $\varphi = q \cdot r$ where $\mathbf{r}$ is the atomic position using $(\mathbf{S} - \mathbf{S}_0)/\lambda = \mathbf{H}_{hkl}$ for a diffraction event ($\mathbf{H}_{hkl} = h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3$).

e) The amplitude of a diffracted wave is calculated using this phase angle, φ, and the expression:

$$A = \sum_{AllAtoms\,in\,UnitCell} A_{Atom} e^{-i\varphi}$$

Where the summation is over all atoms in the unit cell. In amorphous materials the atoms are no longer at discrete positions [uvw] but follow a continuous distribution function, p($\mathbf{r}$).
Write a similar expression relating the amplitude of a diffracted wave at wave vector $\mathbf{q}$ to the continuous distribution function p($\mathbf{r}$).

Answers: Quiz 6 XRD 5/4/01

a) $\varphi = 2\pi(hu + kv + lw)$

$$\varphi = 2\pi\left(H_{hkl} \cdot r_{uvw}\right) = 2\pi\left(\left(hb_1 + kb_2 + lb_3\right) \cdot \left(ua_1 + va_2 + wa_3\right)\right)$$

and the only components that have a value are where $\mathbf{a}_i \mathbf{b}_i = 1$

b) The diffraction angle is obtained from Bragg's law using $d^2 = a^2/(h^2 + k^2 + l^2)$ for a cubic system. So the vector H_{hkl} is directly related to the diffraction angle. The crystal unit cell is composed of vectors $\mathbf{r}_{uvw}$. Then the phase relates the unit cell atoms to the diffraction angle.

c) $\mathbf{p} = h\nu/\mathbf{c} = \mathbf{h}/\lambda$.

This is the same as the analysis of **S** vectors in real space except $\mathbf{S}/\lambda$ is replaced with **p**. The result is that $\Delta\mathbf{p} = 2h\sin\theta/\lambda$

$\mathbf{q} = 2\pi\Delta\mathbf{p}/h$

d) From part a we have $\varphi = 2\pi\left(H_{hkl} \cdot r_{uvw}\right)$. From part c we have that $\mathbf{q} = 2\pi(\mathbf{S} - \mathbf{S}_0)/\lambda = \mathbf{H}_{hkl}$.
So, $\varphi = q \cdot r$.

e) $A(q) = A\int p(r) e^{-i(q \cdot r)} dr$

This shows that the amplitude of the diffracted beam is the Fourier transform of the electron distribution function p(r).