061101 Quiz 6 XRD

This week we began consideration of the calculation of the diffracted intensity based on an inverse space vector $\mathbf{H} = h\mathbf{b}_1 + k\,\mathbf{b}_2 + l\,\mathbf{b}_3$ and real space atomic positions $\mathbf{U} = u\,\mathbf{a}_1 + v\,\mathbf{a}_2 + w\,\mathbf{a}_3$. The reciprocal space vector $\mathbf{H}$, is connected to the Bragg angle 2θ through Bragg's law and equations for the d_{hkl}-spacing.   The real space atomic position, $\mathbf{U}$, is connected to the crystallographic structure and orientation relative to the incident x-ray.

1) Give an expression that describes the structure factor, F_{hkl}, for a crystal with N atoms at positions u_i, v_i, w_i. (This involves a sum of complex exponentials.)

2) For an FCC structure show that this expression yields 4f for hkl unmixed and 0 for hkl mixed.

3) The Thompson function describes diffraction from a single free electron. What is a single free electron and why is the diffraction from a single free electron important to the calculation of diffraction from a block of copper using partially polarized x-rays such as in the diffractometer used in the lab?

4) The multiplicity factor, p, for {111} is 8 while for {110} is 12. What is the multiplicity factor and why does it differ for these two types of planes (show how values of 8 and 12 can be obtained)?

5) For the brass key run in the lab this week we use Vergard's law to determine the zinc/copper content. Would you expect orientation of the crystals in this processed sample to effect the results? What if the key contained a coating of chrome and we wanted to determine the amount of chrome in the key?

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1) $F_{hkl} = \sum_{i=0}^{N-1} f \exp\left(-i2\pi\left(hu_i + kv_i + lw_i\right)\right)$

2) For FCC there are 4 atoms per unit cell: [0 0 0]; [1/2 1/2 0]; [1/2 0 1/2]; [0 1/2 1/2], yielding,
$F_{hkl} = f\left(1 + \exp\left(-i\pi(h+k)\right) + \exp\left(-i\pi(h+l)\right) + \exp\left(-i\pi(k+l)\right)\right)$
if h, k, l are unmixed (all even or all odd) then the argument to the exponentials will be all even since the sum of two odds is even and the sum of two evens is even. Given that $\exp(-in\pi) = (-1)^n$, even powers will result in $F_{hkl} = f(1+1+1+1) = 4f$. For mixed Miller indicies, one argument will always be even (two odds or two even) and the other two will be odd (sum of one odd and one even). Then the structure factor is $F_{hkl} = f(1+1-1-1) = 0$ so these peaks will not be observed.

3) A single free electron is an isolated electron in free space, i.e not bound to an atom and dilute so there is no interference with other electrons. This is the building block for construction of the diffracted x-ray intensity from any material. We consider the scattering from an electron, then interference in the atom, atomic form factor, then interference between atoms, crystallographic structure factor and finally how the crystals are put together in the sample, i.e. the block of copper. For unpolarized x-rays the Thompson factor yields the Lorentz polarization factor $(1 + \cos^2 2\theta)$. For partially polarized x-rays we need to consider the degree of polarization, $\cos^2 2\alpha$ for a crystallographic monochromator for instance. Then the Lorentz factor becomes $(1 + \cos^2 2\alpha \cos^2 2\theta)$.

4) The multiplicity factor, p, reflects the number of indistinguishable planes in a unit cell. This number is different for different planes so a plane with many indistinguishable types in a unit cell will have a relatively higher diffracted intensity compared to planes with fewer indistinguishable types. For {111} the normal to these planes point to the corners of the unit cell so there are 8 indistinguishable (111) planes in a cubic unit cell. For {110} the normal to these planes point to the edges of the unit cell so there are 12 of these planes in a cubic unit cell.

5) Orientation will effect the relative intensity of diffraction lines, but since Vergrad's Law does not use the relative intensity but the d-spacing, it is not sensitive to orientation as long as the diffraction peak can be observed. Determination of the amount of chrome will involve comparison of peak intensity similar to the Moly/Copper measurement and will certainly depend on orientation of the crystals in the processed key.