041015 Quiz 3 X-ray Diffraction

a) Sketch an FCC lattice showing (111), [010] and <110>. (Label these; include 2 examples in the family)

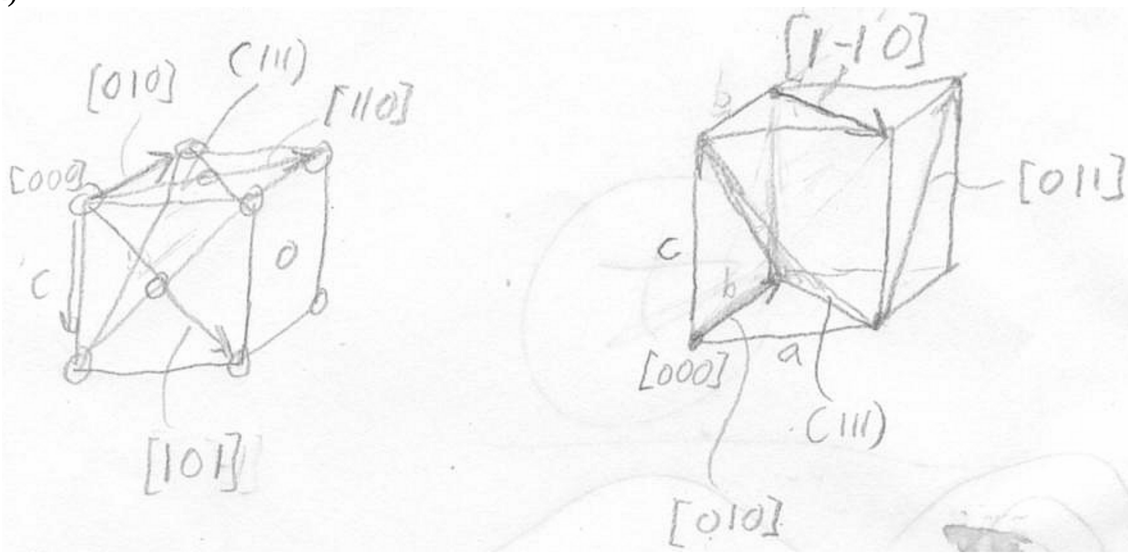
b) Explain how (111) in an FCC lattice; is related to (0001) in a hexagonal closest packed lattice ((001) in the tetragonal depiction).

c) NaCl dislays an FCC structure. Sketch the NaCl structure showing a lattice site by drawing a block around the repeat unit.

d) Explain how {110} and {100} can be planes of a zone. (You will need to explain what "planes of a zone" are and you will need to calculate the zone axis. Consider specifically (110) and (100); and (110) and (001). It may be helpful to sketch the unit cell.)

e) In lab we have used two methods to describe crystallographic orientation in a processed sample such as a wire or sheet, the pole figure and the Hermans orientation function. Describe in (2 sentences each) these two methods and comment on their comparative usefulness (2 sentences each).

a)



b) (111) is a hexagonal plane in the FCC structure. These planes stack in an ABCABC… motif in FCC. If the stacking is changed to ABABAB… the (111) becomes (0001) in the hexagonal closest packed lattice. The (111) in FCC is indistinguishable from (0001) in the HCP if only that plane and one nearest neighbor plane are considered.

c)

There is also a Cl in the middle of the unit cell.

d) Planes of a zone are planes with a coincident in plane vector which is the zone axis. If a plane is in a zone the zone axis [uvw] and the plane normal [hkl] are normal so that the dot product of the two vectors equals 0. That is uh + vk + wl = 0. By inspection it can be seen that [001] is a zone axis for planes of the type (110) and (100). For the two planes (110) and (001) the zone axis can be calculated using,

$u = k_1 l_2 - k_2 l_1$
$v = l_1 h_2 - l_2 h_1$

$w = h_1k_2 - h_2k_1$

which yields [1 -1 0] as a zone axis. This could also be obtained by inspection.

e) The pole figure is a stereographic projection that compares the sample frame of reference to the crystallographic plane of reference for a single plane in terms of a probability distribution mapping. The Hermans orientation function is calculated from the average projection of a plane normal in the machine direction a function which varies from 0 to 1 (like a weight fraction orientation) using a Legendre polynomial. The Hermans function is the most commonly used description of orientation but it assumes axial symmetry (fiber orientation).

The Hermans function gives an analytic description of orientation but ignores the 3 dimensionality of orientation in favor of a simple value based on fiber symmetry. The pole figure gives a qualitative description of orientation in 3 dimensions but does not yield a simple analytic value.