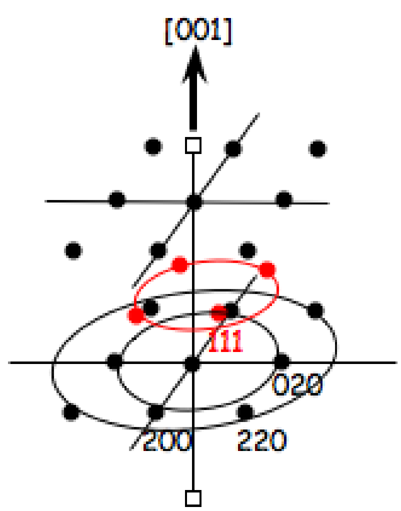
1. An almost infinite number of tiny, perfectly cube-shaped grains of salt, about 1 micron in size, are dropped onto a flat glass plate so that they are extremely densely packed. For NaCl, a = 5.64 Å.

   Construct, to scale, a drawing of the representation of the reciprocal lattice for this specimen, index, and explain.
   (You did this before.)

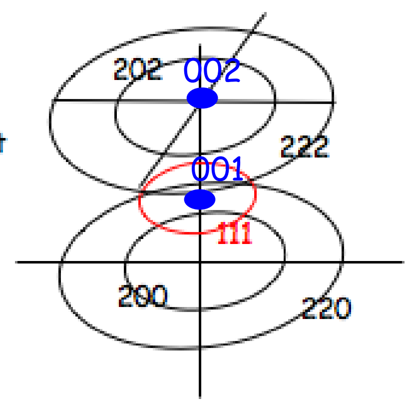
   Now make the glass plate + NaCl crystals the specimen in a powder diffractometer. Do the Ewald construction (CuKα radiation) for such a specimen to see what the powder pattern would look like. Draw and describe the pattern.

   From the last problem set:



Answer;

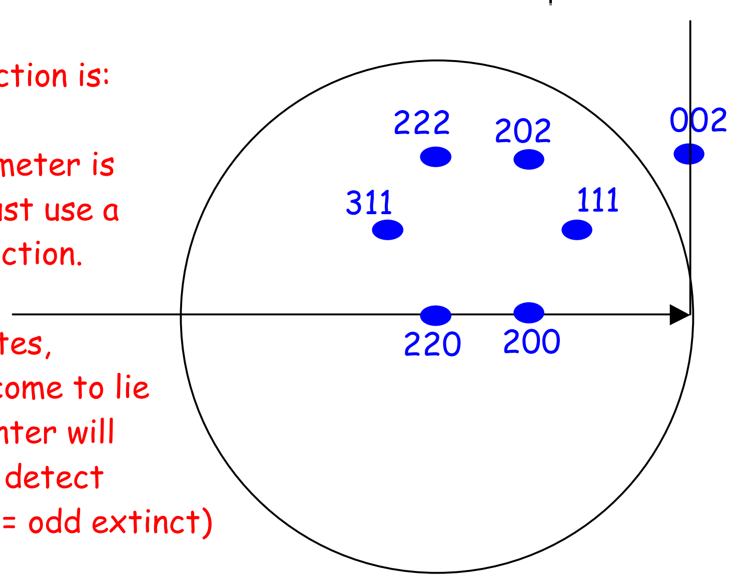
(rings repeat along [001])

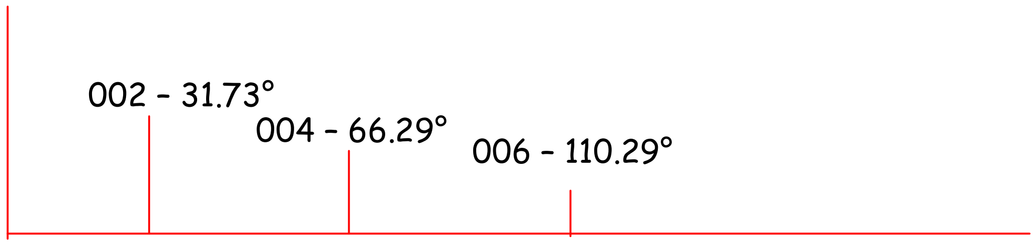


Now, the Ewald construction is:

Since powder diffractometer is a 2-D instrument, can just use a circle for Ewald construction.

As diffractometer rotates, many of the points will come to lie on Ewald circle, but counter will only be in right place to detect (00l) reflections (with l = odd extinct)



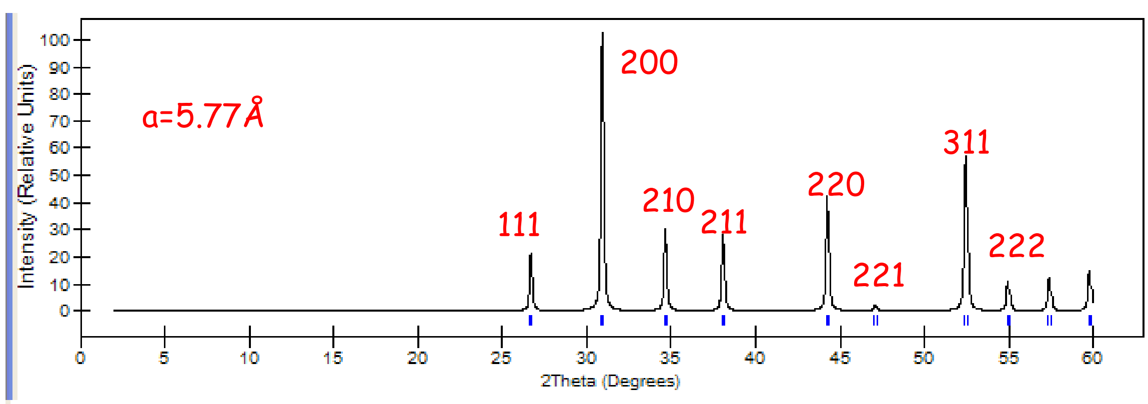


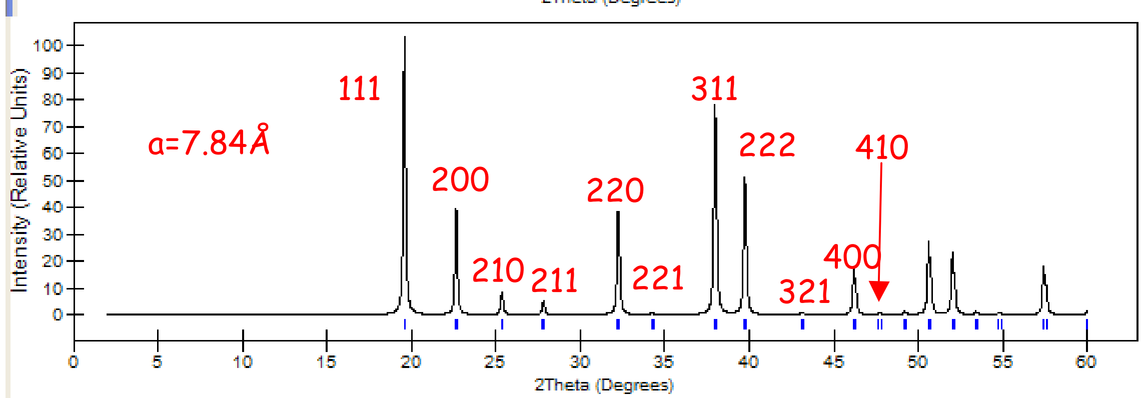
2. Determine the angle settings (crystal angle and counter angle) for a graphite monochromator for FeKa radiation.

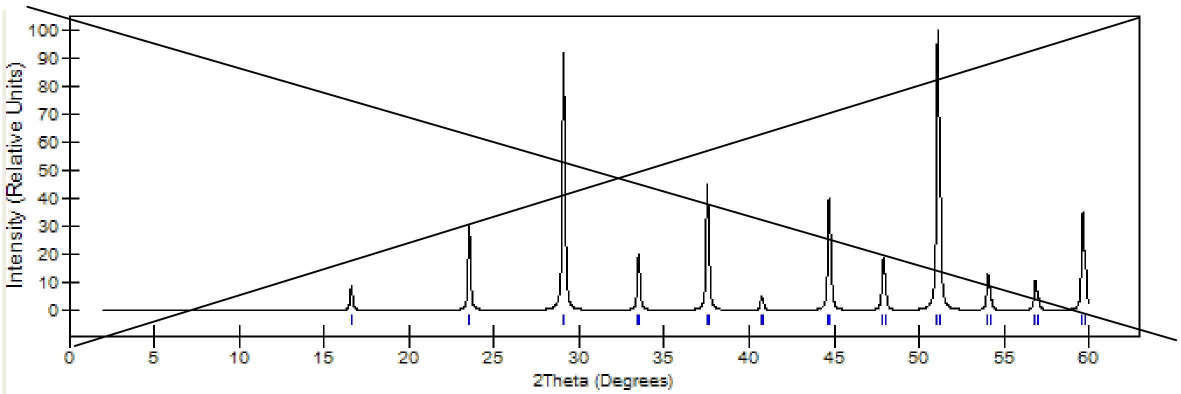
   $c = 2d_{002} = 6.708$ Å $\lambda/2d_{002} = \sin\theta_{002}$

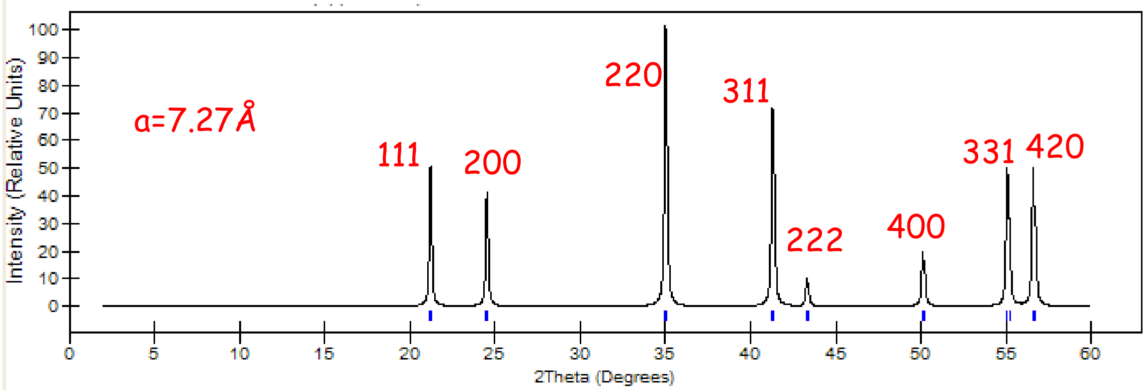
   $1.937355/6.708 = 0.2888 = \sin\theta_{002}$; $\theta = 16.78°$, $2\theta = 35.57°$

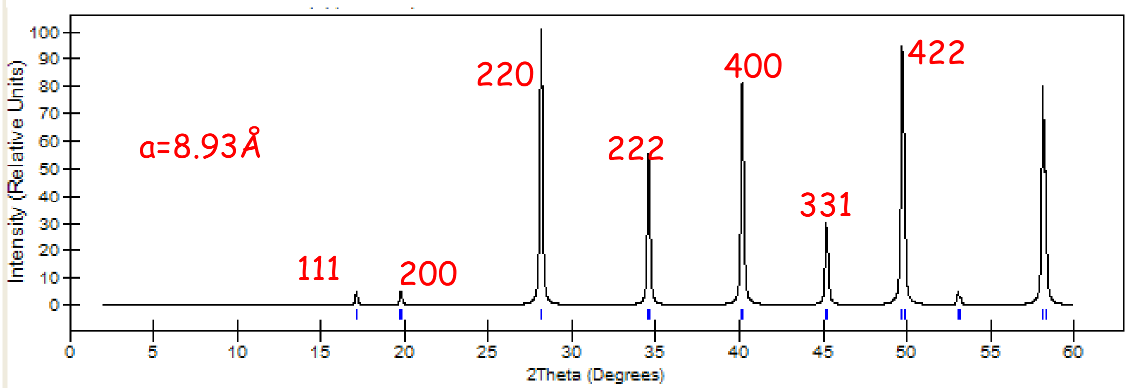
3. Index these patterns and calculate approximate lattice parameters for each material. (CuKα radiation)

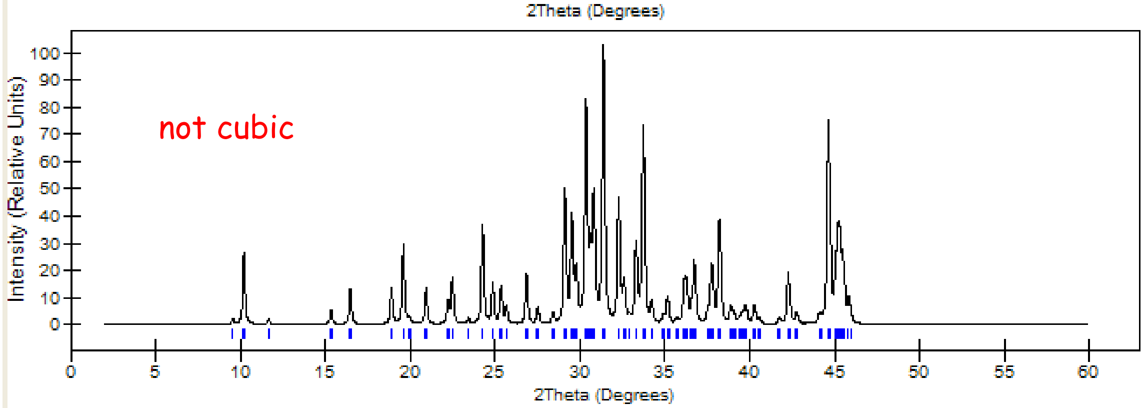












4. Derive the extinction rule for C-centering by calculating which (hkl)s systematically have F = 0. Follow the procedure discussed for I-

centering in class. State the rule in the same form as that given in class.

For every atom at (x,y,z) there must be one at ($x + \frac{1}{2}, y + \frac{1}{2}$,z)

Then:

$$F = \sum_{j=1}^{N/2} f\,(\exp(2\pi i\,(hx_j + ky_j + lz_j)) + \exp(2\pi i\,(h(x_j+1/2) + k(y_j+1/2) + lz_j)))$$

Breaking exponents apart, and reassembling:

$$F = \sum_{j=1}^{N/2} f\,(\exp(2\pi i\,(hx_j + ky_j + lz_j))\,(1 + \exp(\pi i\,(h + k)))$$

rule: (hkl), h + k = 2n (even)

5. Derive the extinction rule for a 2_1 screw axis in monoclinic by calculating which (hkl)s systematically have F = 0. For this screw axis, for every atom at (x_j, y_j, z_j), there must be a symmetry-equivalent atom at ($-x_j, y_j + 1/2, -z_j$). State the rule in the same form as that given in class.

For every atom at (x,y,z) there must be one at ($-x, y + \frac{1}{2}, -z$)

Then:

$$F = \sum_{j=1}^{N/2} f\,(\exp(2\pi i\,(hx_j + ky_j + lz_j)) + \exp(2\pi i\,(-hx_j + k(y_j+1/2) - lz_j)))$$

Can't do anything to reduce this unless h,l = 0. Then:

$$F = \sum_{j=1}^{N/2} f\,(\exp(2\pi i\,(hx_j + ky_j + lz_j))(1 + \exp(\pi i\,k))$$

rule: (0k0), k = 2n