MTSE 3010 (Bonding and Structure) Homework 4 - DUE 12/3/2019 (in class)

1. (a) List two planes that belong to the hexagonal zone [1121].

(b) Find the plane which lies parallel to the directions [131] and [011]. Find the direction which lies parallel to the intersection of the planes (213) and (110). Check your answers by using the Weiss zone law.

2. The high-pressure form of Te has a=3.104, b=7.513, c=4.766Å, β=92.71° and α=γ=90°. Te_I is in 2a, x=0.25, y=0.23, z=0.48 and Te_II is in 2a, x=0.48, y=0.00, z=0.02.

   2a = (x, y, z); (x, y, 1/2 + z)

   (a) Present a drawing, roughly to scale, which shows the positions of all the atoms in the unit cell in projection down the c-axis. At the side of the drawing, list the coordinates for all the atoms; mark the z (only the z) coordinates next to all the atoms on the diagram. Label all the lattice parameters in your cell.

   (b) Is the structure centric? Why?

   (c) Determine the structure factor (F_{hkl}) for this randomly orientated material with minimal crystal imperfection.

   (d) For a value of S=1 you would observe in XRD, what are the values of F_{hkl} (leave your answers in terms of atomic scattering factors)? Recall that for monoclinic crystal system a≠b≠c thus (100)≠(010)≠(001) reflections will have different plane spacings (d-spacings) and thus F_{hkl} values. Note about calculations: if you calculate for example 0.1456 + -0.1423 = 0.0033, we treat this as essentially = 0.

   (e) Based on your answer in (d) for S=1, are all reflections possible? Why or why not?

   (f) Calculate the XRD intensities for S=1 assuming λ=1.54 Å. LP=(1+cos^22θ)/sin^2θcosθ

   (g) Even without calculating the XRD intensities, would you expect the (010) or the (001) to have the highest XRD intensity (explain how you determined your answer)?

3. Mica is C2/m with a=5.208 Å, b=8.995 Å, c=10.275Å, and β=101.6°. Assume that the mica sheets are parallel to the (00l) “L not 1” planes. Calculate the 2θ’s (to two decimal places) for all of the geometrically possible reflections which occur for CrKα radiation (λ=2.2910Å).