Tutorial VI (2011- 2012 Sem II) Prof A K Ganguli : Course Coordinator Powder X-ray Diffraction

1. Using diffraction from a set of planes deduce Bragg's Law

2. Explain the difference between a filter and a primary monochromator

3. Explain how the d – values are calculated from the Debye-scherer film.

4. The d-spacing for the 110 planes of a metal crystallizing in the cubic structure is equal to 2.952 A. Calculate the d- spacing corresponding to the 111 and 311 planes.

5. Calculate the cell parameters of a tetragonal cell which shows the following d – values; $d_{110} = 2.828$; $d_{020} = 2.000$; $d_{201} = 1.897$ Å

6. Given the powder x-ray diffraction pattern, index the reflections on a cubic cell and calculate the lattice parameters. (d-values given).



7. Give the important parts of a powder diffractometer.

8. Write brief notes on a) scintillation detector and 2) CCD detector

9. What is the difference between a theta-theta and theta-2theta goniometer.

10. In what type of crystalline materials would you see preferred orientation effects in the diffraction patterns?

11. How do you obtain the crystallite size of particles usig X-ray diffraction?

12. The powder x-ray diffraction pattern (a) of a sample was collected on a diffractometer A at room temperature. The sample gave a diffraction pattern (b) when it was heated to high temperature and the data was collected using the same diffractometer A. The initial sample when recorded on a different diffractometer B gave the pattern (c) at room temperature. What are the possible reasons for the differences among (a), (b) and (c) ?



13. Given the following electron diffraction photographs of an oxide sample at 373K and 1273K.



(a) what are the hkl values for the spots marked with an arrow?

(b) Given $\mathbf{a} = 4A$ at 373K what is the value of \mathbf{a} and \mathbf{a}^* at 1273K

14. What information you can derive from powder diffraction patterns of a solid sample? Sketch the diffractograms of a glass, layered aluminosilicate like mica, and NaCl. Give the possible indices of the peaks wherever possible.