

1. Diffraction powder analysis

Specimens of three different monatomic cubic crystals are analyzed using the powder method and peaks are found in the x-ray spectra at the following angles. One of the crystals is fcc, one is bcc and one has the diamond structure. Note that angle between the scattered \vec{k}' and incident wavevector \vec{k} is given in the table.

A	B	C
44.2°	28.8 °	42.8°
49.2	41.0	73.2
72.0	50.8	89.0
87.3	59.6	115.0

- Identify the crystal structure of A,B and C.
- If the wavelength of the incident X-ray beam is 1.54 Å, what is the length of the side of the conventional cube in each case ?
- If the diamond structure were replaced by a cubic zinc sulfide structure with a cubic unit cell of the same side, at what angles would the first four lines in the pattern now occur?

2. Powder Diffraction of *hcp* and *fcc* crystals

Cobalt has two forms: α -Co, with *hcp* structure (in-plane atomic spacing of $a=2.51$ Å and β -Co, with *fcc* structure (lattice spacing of $a_{cubic}=3.55$ Å). Note that for a has different meanings in α and β structures. Assume that the *hcp* structure has the ideal c/a ratio. Calculate and compare the angles (2θ) of the first five X-ray diffraction peaks assuming Cu $K\alpha$ radiation where $\lambda = 1.54\text{Å}$ is used.

3. Effect of Cubic-Tetragonal Transition on powder x-ray pattern

CuV_2S_4 is a material that is cubic at 300 K but undergoes a transformation from a cubic to a tetragonal bravais lattice at 90 K . For T just above 90 K the cubic lattice parameter $a=9.788$ Å. Just below the transition temperature $a=9.793$ Å and $c=9.775$ Å. Determine the diffraction angles θ of the (100), (110), (111), (200) and (120) peaks in the cubic powder xray diffraction pattern and the splitting of these peaks in the tetragonal phase. Assume $\lambda = 1.54$ Å.