

Oxford Neutron Summer School Tutorial Questions – J.P. Attfield

1. A spinel, Co_2FeO_4 is studied by neutron diffraction to determine the proportions of Co and Fe at the octahedral and tetrahedral cation sites. The relative scattering lengths of the octahedral, tetrahedral and oxygen sites are found to be in the ratio 1: 0.45: 0.95. Calculate the proportions of Co and Fe at the two cation sites. Why could X-ray diffraction not be used to derive this information?

[Elemental scattering lengths O 5.80, Fe 9.45, Co 2.49 fm]

2. (i) What useful information about a crystalline material is derived from:

(a) positions

(b) intensities

(c) widths

of diffraction peaks in a Rietveld refinement?

(ii) The three longest-d peaks in the neutron powder diffraction pattern of a primitive tetragonal material have d-spacings of $d = 5.60, 4.12$ and 3.96 \AA . Derive the Miller indices for these three reflections and the unit cell parameters of the material.

(iii) When the above material is cooled, the 5.60 \AA peak splits into two peaks of approximately equal intensity but the 4.12 and 3.96 \AA peaks do not split. What lattice distortion does this signify?

[Information: a tetragonal unit cell has dimensions $a = b \neq c$, angles $\alpha = \beta = \gamma = 90^\circ$]