

Question B1: The intensity of a line is given by

$$I(\theta) = MG(\theta)F_{hkl}F_{hkl}^*$$

M is the multiplicity, e.g M=6 for 100 in cubic crystals. F_{hkl} is the structure factor given by

$$F_{hkl} = \sum_j f_j \exp(-i2\pi \mathbf{r}_j \cdot \mathbf{g}_{hkl})$$

where the sum is over all the atoms in the motif. It depends on the content of the unit cell. f is θ dependent because of the nature of the scattering (X-rays scattered by electrons around nucleus).

In the first case, the sequence of permitted reflections indicates a cubic I structure (all $h + k + l$ odd are absent). Given the size of Cu and Zn and the lattice parameter, the cell will contain a maximum of one of each of these atoms. Since the structure is disordered, we can describe it by attributing a 50% probability to find either of both atoms on each lattice point. So that the motif can be written:

$$\begin{aligned} 000 & : 0.5\text{Cu}, 0.5\text{Zn} \\ \frac{1}{2} \frac{1}{2} \frac{1}{2} & : 0.5\text{Cu}, 0.5\text{Zn} \end{aligned}$$

When ordering occurs, the new motif is:

$$\begin{aligned} 000 & : \text{Cu} \\ \frac{1}{2} \frac{1}{2} \frac{1}{2} & : \text{Zn} \end{aligned}$$

Note that there is no importance whatsoever which one you chose to place on [000]

The structure factor of the cubic P is, in general:

$$F_{hkl} = f_{\text{Cu}} + f_{\text{Zn}} \exp(i\pi(h+k+l))$$

from which it is immediate that:

$$\begin{aligned} F_{hkl} & = f_{\text{Cu}} + f_{\text{Zn}} \text{ if } h+k+l \text{ even} \\ F_{hkl} & = f_{\text{Cu}} - f_{\text{Zn}} \text{ if } h+k+l \text{ odd} \end{aligned}$$

which explains why 100 or 111 reflections are much weaker than 110 or 200 etc..

When we consider a 30wt% Zn, 70wt% Cu mixture, the first thing is to identify the phase(s) you would expect a mixture of such composition to form. A quick look at your data book should tell you that there is a single phase (Cu) which is a solid solution of Zn in Cu and hence is ccp. The diffraction pattern will therefore show only the reflections for hkl all odd or all even.