Problems Sheet for lectures 9 and 10

1) Show that the spacing d between the $(hk\ell)$ planes in a cubic lattice of side a is

$$d = \frac{a}{\left(h^2 + k^2 + \ell^2\right)^{1/2}}$$

2) (a) For a simple cubic lattice with cube side a, write down the Miller indices for the eight most widely spaced sets of planes that give rise to Bragg reflections, and calculate the spacings of the planes for each case.

(b) Repeat question 1 for a body-centred cube having the same conventional cube size – you need only write down the first seven.

(c) ... and for a face-centred cube, write down the first five.

(d) In an x-ray diffraction experiment to determine the structure of a crystal for which a is unknown, monochromatic x-rays are used, and a set of Bragg angles determined, θ_1 to θ_8, corresponding to diffraction from most widely spaced sets of planes having spacings d_1 to d_8. These are related by:

$$\sin\theta_1 : \sin\theta_2 : \sin\theta_3 : ... = \frac{1}{d_1} : \frac{1}{d_2} : \frac{1}{d_3} : ...$$

Show that only the first two Bragg angles are required to distinguish between a simple cubic and face-centred cubic structure, but that seven are required to distinguish between simple cubic and body-centred cubic.

3) The diamond structure is face-centred cubic with a 2-atom basis at (000) and (1/4 1/4 1/4) (using conventional cubic co-ordinates). Determine the Miller indices of the four most widely spaced sets of planes that give rise to Bragg reflections in diamond. [Hint: the fcc lattice leads to restrictions on the Miller indices – see question 1. The structure factor of the 2-atom basis then leads to further restrictions.]

4) Repeat question 2, but treating the diamond structure as a simple cubic structure with an 8-atom basis. [Hint: the restrictions on the Miller indices now come entirely from the structure factor.]

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