Problem A& M 6.1

First make sure you understand Equation 6.12 in A&M (pp 103-104). It shows that the planes corresponding to the smallest reciprocal lattice vector yield the smallest angle for the ring. Thus we know that the angle at which the j^{th} diffraction ring occurs is determined by the ratio

$$\frac{\sin(\phi_j/2)}{\sin(\phi_1/2)} = \frac{d_j}{d_1}$$

where d_j is the magnitude of the the j^{th} reciprocal lattice vector arranged according to increasing magnitudes.

Since we need the lengths of the reciprocal lattice vectors we do that first. This is easy since the reciprocal lattice of the fcc lattice is bcc and vice versa. So we just need to find the distances in these lattices in real space.

bcc lattice: The lattice sites arranged in order from the origin have coordinates $(0,0,0)$, $(1/2,1/2,1/2)$, $(1,0,0)$, $(1,1,0)$, $(3/2,1/2,1/2)$,$(1,1,1)$, $(2,0,0)$ and their symmetry counterparts. The distances from the origin are

$$\frac{\sqrt{3}}{2},\ 1,\ \sqrt{2},\ \frac{\sqrt{11}}{2},\ \sqrt{3},\ \ 2$$

which yields the ratios

$$1 : \frac{2}{\sqrt{3}} : \frac{2\sqrt{2}}{\sqrt{3}} : \frac{\sqrt{11}}{\sqrt{3}} : 2 : \frac{4}{\sqrt{3}} \ = \ 1 : 1.1547 : 1.63299 : 1.91485 : 2 \ : \ 2.3094.$$

fcc lattice: The lattice sites arranged in order from the origin have coordinates (other than the origin) $(1/2,1/2,0)$, $(1,0,0)$, $(1,1/2,1/2)$, $(1,1,0)$,$(3/2,1/2,0)$, $(1,1,1)$ whose distance from the origin are $1/\sqrt{2}$, 1, $\sqrt{3}/\sqrt{2}$, $\sqrt{2}$, $\sqrt{5}/\sqrt{2}$, $\sqrt{3}$. The ratios are

$$1 : \sqrt{2} : \sqrt{3} : 2 : \sqrt{5} : \sqrt{6} \ = \ 1 : 1.41421 : 1.73205 : 2.0 : 2.23607 : 2.44949\,.$$

For sample A the ratios are easily computed:

$$1 : 1.156 : 1.63 : 1.917$$

and thus the reciprocal lattice is *bcc* and the direct lattice is *fcc*.
Similarly, for sample B the ratios of the sines are computed to be

$$1 : 1.141 : 1.72 : 2.00$$

identifying the reciprocal lattice to be *fcc* and the direct lattice to be *bcc*.

The third sample is thus deduced to be the diamond lattice; we can check this by looking at the missing rings: The diamond lattice is an fcc lattice with a basis of two

atoms at $\vec{d_1} = (0, 0, 0,)$ and $\vec{d_2} = a(1/4, 1/4, 1/4)$. The reciprocal lattice is a bcc lattice with primitive vectors

$$\vec{b}_1 = \frac{2\pi}{a}(-\hat{x} + \hat{y} + \hat{z}), \quad \vec{b}_1 = \frac{2\pi}{a}(\hat{x} - \hat{y} + \hat{z}), \quad \vec{b}_1 = \frac{2\pi}{a}(\hat{x} + \hat{y} - \hat{z}), \quad .$$

Thus the structure factor is

$$e^{i\vec{G}\cdot\vec{d}_1} + e^{i\vec{G}\cdot\vec{d}_2} = 1 + e^{i\frac{\pi}{2}(h+k+\ell)}.$$

This clearly implies that if $h + k + \ell$ is an *twice an odd* integer the structure factor vanishes. Thus some of the peaks must be missing. The second peak with ratio 1.1547 corresponding to (110) is missing; the fifth peak corresponding to $(2, 0, 0)$ with the ratio 2 should also be missing. Indeed they are if one computes the ratios from the data given in A&M.

Note that if diamond is replaced by the zincblende structure the exact extinction of the (110) , $(2, 0, 0)$, and $(2, 2, 2)$ planes no longer occurs since the charge form factors of the two atoms can be different. Thus new rings are introduced at angles that can be calculated: one is at 49.6°.