MASSACHUSETTS INSTITUTE OF TECHNOLOGY

Physics Department

8.231, Physics of Solids I — Due on Sept. 18

Problem set #2

1. X-ray Powder diffraction

   X-ray powder diffractions are done for three crystals. Each crystal is formed by one find of atoms. The atoms in the three crystals form a simple cubic (SC), a face centered cubic (FCC), and a body centered cubic (BCC) crystal structures respectively. Let ϕ be the diffraction angle. The diffraction peaks are observed at the following diffraction angles for the three crystals:

$$\text{Crystal A: } \sin\frac{\phi}{2} = 0.127,\ 0.180,\ 0.255,\ 0.285,\ 0.312.$$

$$\text{Crystal B: } \sin\frac{\phi}{2} = 0.150,\ 0.212,\ 0.260,\ 0.300,\ 0.335,\ 0.367.$$

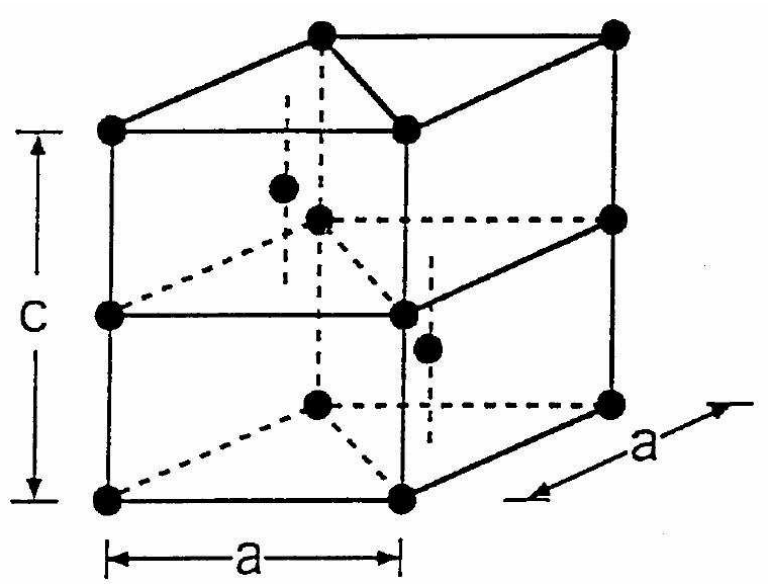
$$\text{Crystal C: } \sin\frac{\phi}{2} = 0.121,\ 0.140,\ 0.198,\ 0.232,\ 0.242,\ 0.280,\ 0.305.$$

   (a) Identify the crystal structures of the crystal A, B, and C.

   (b) Sketch the first four powder diffraction peaks for the SC crystal. Now assume that as we lower the temperature, the SC crystal is changed into the tetragonal structure through a continuous phase transition. Describe and sketch how the above four peaks change as the crystal changes into the tetragonal structure.

2. Americium

   The figure below shows a primitive unit cell of one crystalline form of the element Americium. The space lattice is hexagonal with $\vec{a_1} = a\hat{x}$, $\vec{a_2} = \frac{1}{2}a\hat{x} + \frac{\sqrt{3}}{2}a\hat{y}$, and $\vec{a_3} = c\hat{z}$. The basis is (000), $(\frac{2}{3}\frac{2}{3}\frac{1}{4})$, $(00\frac{1}{2})$, and $(\frac{1}{3}\frac{1}{3}\frac{3}{4})$.



(a) Find the reciprocal lattice vectors $\vec{G}$. Describe in words and sketch the reciprocal lattice.

(b) Find the structure factors associated with the points (100), (001), and (120) of the reciprocal lattice.

(c) Calculate the three smallest X-ray diffraction angles in a powder diffraction experiments. Assuming $c = 2a$ and the wave length of the X-ray to be $\lambda = a/10$.

3. Form Factor for Atomic Hydrogen

   For the hydrogen atom in its ground state, the number density is $n(r) = (\pi a_0^3)^{-1} \exp(-2r/a_0)$. where a_0 is the Bohr radius. Show that the form factor is $f_G = 16/(4 + G^2 a_0^2)^2$.

4. Reciprocal Lattice of Conventional versus Primitive Unit Cells

   (a) Why are there fewer reciprocal lattice points $\vec{G}$ in a given volume of Fourier space if the unit cell of the crystal lattice is primitive than if the unit cell is non-primitive?

   (b) In view of (a), how can the allowed reflections from a given structure be independent of the choice of the unit cell of the crystal lattice?