Work Sheet # 3

1. Find the distribution of atoms in the atomic planes (010), (110) and (111) of a simple cubic crystal structure.

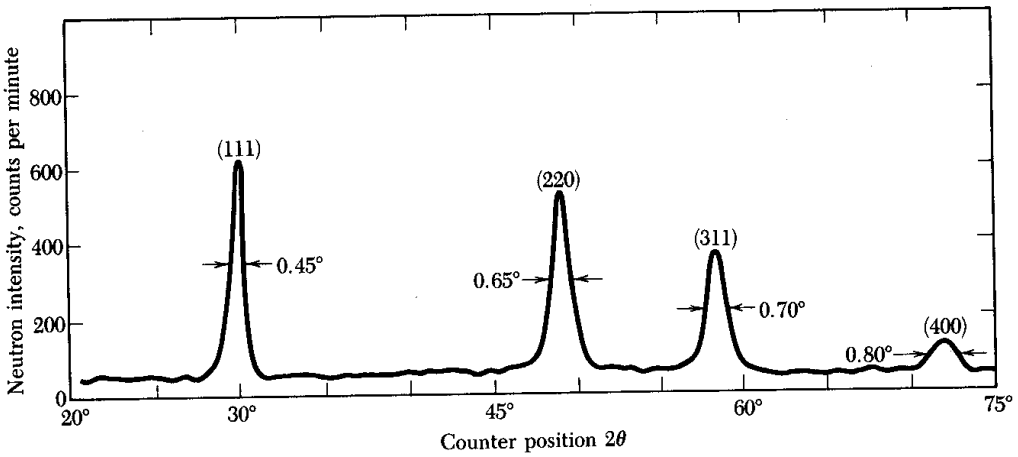
2. Prove that the lattice planes with the greatest densities of points are the {111} planes in a face-centered cubic Bravais lattice and the {110} planes in a body-centered cubic Bravais lattice.
[Hint: (1) This is most easily done by exploiting the relation between families of lattice planes and reciprocal lattice vectors. (2) Take the primitive vectors for fcc lattice as: $\vec{a}_1 = \frac{a}{2}(\hat{y}+\hat{z})$, $\vec{a}_2 = \frac{a}{2}(\hat{x}+\hat{z})$ and $\vec{a}_3 = \frac{a}{2}(\hat{y}+\hat{x})$].

3. Show that the expression $d(hk\ell) = \frac{2\pi}{|\vec{G}|}$ can be rewritten as *2 d sin* $\theta = n\lambda$, where θ is the angle between the incident beam of x-radiation and the crystal plane.

4. Find the structure factor for an fcc crystal structure when the scattering peaks are indexed to a simple cubic lattice.

5. The number density of the hydrogen atom in its ground state is given by $n(r) = \frac{e^{-2r/a_\circ}}{\pi a_0^3}$, where $a_\circ$ is the Bohr radius. Show that the form factor is $f_G = \frac{16}{(4+G^2a_\circ^2)^2}$.

6. The neutron diffraction pattern for powdered diamond is in figure shown. Find:
   a) The structure factor of the basis of the conventional cell of diamond.
   b) Show that the allowed reflections of the diamond structure satisfy $h + k + \ell = 4n$, where all indices are even and n is an integer, or else all indices are odd.
   c) The zeros of structure factor.



7. Consider a simple cubic crystal structure with a cube edge a= 3.5 $\overset{o}{A}$ and suppose it is used to scatter 3.1 $\overset{o}{A}$ x-rays.
   a) Find all sets of planes that satisfy the Bragg condition and for each peak.
   b) *Find the Bragg angle.*

The followings are MCQ's. Please choose the correct answer:

8. If the wave function of the hydrogen atom in its ground state is given by $\psi(r) = \dfrac{e^{-r/a_\circ}}{a_\circ\sqrt{\pi a_\circ}}$, (where $a_\circ$ is the Bohr radius) the number density of the hydrogen atom must have the form

a. $n(r) = \dfrac{e^{-r/a_\circ}}{a_\circ\sqrt{\pi a_\circ}}$ b. $n(r) = \dfrac{e^{-r/2a_\circ}}{2\pi a_0^2}$ c. $n(r) = \dfrac{e^{r/2a_\circ}}{2\pi a_0^2}$

d. $n(r) = \dfrac{e^{2r/a_\circ}}{\pi a_0^3}$ e. $n(r) = \dfrac{e^{-2r/a_\circ}}{\pi a_0^3}$.

9. Given two identical atoms of the body-centered-cubic (bcc) basis which are located at $(x_1,y_1,z_1) \equiv (0,0,0)$ and $(x_2,y_2,z_2) \equiv (1/2, 1/2, 1/2)$. If the structure factor S_G can be expressed in terms of the form factor of an atom, f, as $S_G(hk\ell) = f(1+e^{-i\pi(h+k+\ell)})$, then the peak intensities that can be observed by x-ray diffraction, are for the planes:

a. (100) and (311)

b. (200) and (110)

c. (221) and (100)

d. (111) and (210)

e. (111) and (414)

10. The intensity peaks of the face-centered-cubic and body-centered-cubic structures are usually indexed using
    a. special kind of vectors called reciprocal vectors of first kind.
    b. the conjugate of reciprocal vectors.
    c. complex cubic lattice vectors.
    d. simple cubic lattice vectors.
    e. special kind of vectors called reciprocal vectors of second kind.