Assignment 2: Diffraction from the Crystal

1. Show that the fcc has the bcc lattice as its reciprocal lattice and vice versa.

2. Diamond has the $Fd\bar{3}m$ space group.
   (a) Find the F.T. of the lattice.
   (b) Find the F.T. of the basis.
   (c) Find the F.T. of the atomic arrangement inside the unit cell.
   (d) What are the systematic absences in the diffraction pattern of diamond? For example show that 222 reflection will be absent. Which absences are due to the lattice and which are due to the basis?

3. Iron ($Im\bar{3}m$), $a = 0.2866$ nm, is irradiated with CrK$_\alpha$ X-radiation ($\lambda = 0.2291$ nm).
   (a) Find the indices $hkl$ and $d$-spacings of the planes which give rise to reflections.
   HINT: prepare a table listing the indices and $d$-spacings of the allowed reflecting planes in order of decreasing $d$-spacing and determine the $\theta$ angles of reflection using Bragg’s law.
   (b) What are the systematic absences for a body-centered lattice?

4. The electron density in a hydrogen atom in its ground state is spherically symmetric, and given by

   $$\rho(r) = \frac{e^{-2r/a_0}}{\pi a_0^3},$$

   where $a_0$, the first Bohr radius, has the value 0.53 Å. Compute the atomic scattering factor $f_a$ for hydrogen, and plot it as a function of $s = 2k \sin \theta = 4\pi \sin \theta/\lambda$. Explain physically why the scattering factor is small for back reflection ($\theta = \pi/2$).

5. Show that the volume of reciprocal cell is equal to the inverse of the direct cell.

Due date: Feb. 27, 2013, 8:30 am in the class