Homework 3

Due 2/2/2012

1. [10 points] Fill in each blank with a number.
   a. Take an fcc lattice. If one uses the conventional sc cell for it, then the volume of the sc cell is [ ] times the volume of the primitive cell. If one calculates the reciprocal of the sc lattice, then it is another sc cell. This reciprocal lattice has a unit cell volume that is [ ] times the volume of the unit cell of the reciprocal lattice of the fcc lattice.
   b. Take a trigonal lattice, whose primitive cell volume is V_p. Take a hexagonal lattice as the conventional lattice. The cenventional cell volume is V_H. $V_H = 3V_p$ as we saw in the previous homework. Then, V_H^*/V_p^* = [ ] where the star subscript means the respective reciprocal lattice.

2. [15 points] Provide your answer to the web question: https://griffin.ucsc.edu/forum/question/68/heart-of-diffraction-a-simple-challenge. Note that this longish problem requires a rather short answer [you do not need anything other than what is stated in the question; we leave f as just a number, whose origin we do not need to worry about at all for the purpose of this problem]. All you need is to express the position of the detector relative to "atom" j in terms of $\vec{r}$ and the position $\vec{x}_j$ of the atom j. Here, $\vec{r}$ is the position of the detector relative to a reference atom, which is placed at the origin.

3. [20 points] Kittel 2.4 (see below).

4. [10 points] Kittel 2.5 (see below): Note that the diamond structure is two atom basis + fcc, where the basis atoms can be taken to be at the origin and at $\frac{a}{4}(\hat{x} + \hat{y} + \hat{z})$, where a is the side of the cube.

5. [10 points] Kittel 2.6 (see below)

6. [20 points] Kittel 2.7 (see below)

Kittel problems from chapter 2:

4. ***Width of diffraction maximum.*** We suppose that in a linear crystal there are identical point scattering centers at every lattice point $\boldsymbol{\rho}_m = m\mathbf{a}$, where m is an integer. By analogy with (20), the total scattered radiation amplitude will be proportional to $F = \Sigma \exp[-im\mathbf{a} \cdot \Delta\mathbf{k}]$. The sum over M lattice points is

$$F = \frac{1 - \exp[-iM(\mathbf{a} \cdot \Delta\mathbf{k}]}{1 - \exp[-i(\mathbf{a} \cdot \Delta\mathbf{k})]} ,$$

by the use of the series

$$\sum_{m=0}^{M-1} x^m = \frac{1 - x^M}{1 - x} .$$

(a) The scattered intensity is proportional to $|F|^2$. Show that

$$|F|^2 \equiv F^*F = \frac{\sin^2 \frac{1}{2} M(\mathbf{a} \cdot \Delta\mathbf{k})}{\sin^2 \frac{1}{2} (\mathbf{a} \cdot \Delta\mathbf{k})} .$$

(b) We know that a diffraction maximum appears when $\mathbf{a} \cdot \Delta\mathbf{k} = 2\pi h$, where h is an integer. We change $\Delta\mathbf{k}$ slightly and define ϵ in $\mathbf{a} \cdot \Delta\mathbf{k} = 2\pi h + \epsilon$ such that ϵ gives the position of the first zero in $\sin \frac{1}{2}M(\mathbf{a} \cdot \Delta\mathbf{k})$. Show that $\epsilon = 2\pi/M$, so that the width of the diffraction maximum is proportional to $1/M$ and can be extremely narrow for macroscopic values of M. The same result holds true for a three-dimensional crystal.

5. ***Structure factor of diamond.*** The crystal structure of diamond is described in Chapter 1. The basis consists of eight atoms if the cell is taken as the conventional cube. (a) Find the structure factor S of this basis. (b) Find the zeros of S and show that the allowed reflections of the diamond structure satisfy $v_1 + v_2 + v_3 = 4n$, where all indices are even and n is any integer, or else all indices are odd (Fig. 18). (Notice that h, k, l may be written for v_1, v_2, v_3 and this is often done.)

6. ***Form factor of 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 $f_G = 16/(4 + G^2a_0^2)^2$.

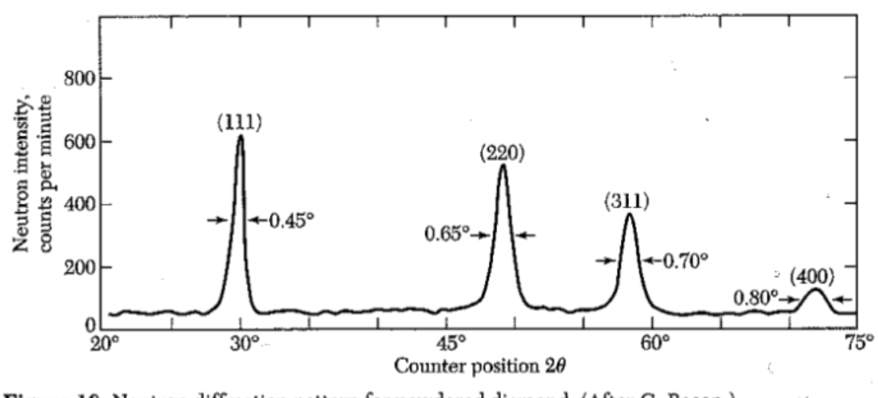

Figure 18 Neutron diffraction pattern for powdered diamond. (After G. Bacon.)

7. ***Diatomic line.*** Consider a line of atoms $ABAB \ldots AB$, with an A—B bond length of $\frac{1}{2}a$. The form factors are f_A, f_B for atoms A, B, respectively. The incident beam of x-rays is perpendicular to the line of atoms. (a) Show that the interference condition is $n\lambda = a \cos\theta$, where θ is the angle between the diffracted beam and the line of atoms. (b) Show that the intensity of the diffracted beam is proportional to $|f_A - f_B|^2$ for n odd, and to $|f_A + f_B|^2$ for n even. (c) Explain what happens if $f_A = f_B$.