Physics 140A Winter 2011

Homework 3 due Wednesday January 26

1. The crystal structure of diamond is described in Chapter 1 of Kittel. 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 add n is any integer, or else all indices are odd. (See Fig. 18 in Kittel Chapter 2). (Notice that h, k, l may be written for v_1, v_2, v_3, and this is often done.)

2. 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 $f_G = 16/(4 + G^2 a_0^2)^2$.

3. Consider a simple cubic crystal with lattice constant 3 Å. A beam of x-rays is incident on the crystal in the $[210]$ direction. For this problem, ignore structure factors.

a) For this geometry, calculate the maximum wavelength for probing the spacing between (110) planes.

b) Assume a detector plate is 10 cm from the crystal. For the wavelength found in part a), sketch the diffraction pattern. (Label distances on the pattern.)

HW 3 Solutions

Note Title 1/20/2010

① Diamond has a fcc lattice with a basis given by 2 atoms for every pt. of the fcc lattice. within the cubic unit cell, we then have:

$$(x_j\, y_j\, z_j) = (0\,0\,0),\ (\tfrac{1}{2}\,\tfrac{1}{2}\,0),\ (0\,\tfrac{1}{2}\,\tfrac{1}{2}),\ (\tfrac{1}{2}\,0\,\tfrac{1}{2})$$
$$(\tfrac{1}{4}\,\tfrac{1}{4}\,\tfrac{1}{4}),\ (\tfrac{3}{8}\,\tfrac{3}{8}\,\tfrac{1}{4}),\ (\tfrac{1}{4}\,\tfrac{3}{8}\,\tfrac{3}{8}),\ (\tfrac{3}{8}\,\tfrac{1}{4}\,\tfrac{3}{8})$$

So the structure factor is:

$$S(v_1 v_2 v_3) = \sum_j f_j \exp\{-i2\pi(v_1 x_j + v_2 y_j + v_3 z_j)\}$$

$$\boxed{\begin{aligned} &= f\Big(1 + \exp\{-i\pi(v_1+v_2)\} + \exp\{-i\pi(v_2+v_3)\} \\ &\quad + \exp\{-i\pi(v_1+v_3)\} + \exp\left(-\tfrac{i\pi}{2}(v_1+v_2+v_3)\right) \\ &\quad + \exp\left\{-\tfrac{i\pi}{2}(3v_1+3v_2+v_3)\right) + \exp\left\{-\tfrac{i\pi}{2}(v_1+3v_2+3v_3)\right) \\ &\quad + \exp\left\{-\tfrac{i\pi}{2}(3v_1+v_2+3v_2)\right\}\end{aligned}}$$

now, the 1st set of terms are just the same as for an fcc lattice, and are zero unless $\underline{v_1, v_2 \text{ \& } v_3 \text{ are all even or odd}}$

next note that $\exp\left\{-\frac{i\pi}{2}(3v_1+3v_2+v_3)\right\}$

$$= \exp\left\{-i\pi(v_1+v_2)\right\}\exp\left\{-\frac{i\pi}{2}(v_1+v_2+v_3)\right\}$$

(and similar expressions for the other 2 terms)

So we must also have $v_1+v_2+v_3 = 4n$ where $n \in \mathbb{Z}$ to make the last 4 terms non-zero.

On the other hand, if $v_1+v_2+v_3 = 2n$ where $n \in \mathbb{Z}$, then there we get a factor of (-1) for the last 4 terms and hence S vanishes

so we have :

allowed : $\left\{ \begin{array}{l} hkl \text{ all odd } \underline{\text{or}} \text{ all even} \\ \underline{\text{and}} \quad h+k+l = 4n \end{array} \right.$

zeros : $\left\{ \begin{array}{l} hkl \text{ are even, even, odd or even, odd, odd} \\ \text{or} \quad h+k+l = 2n \end{array} \right.$

② $$f_G = 4\pi \int_0^\infty r^2 \frac{\sin Gr}{Gr} \frac{1}{(\pi a_0^3)} e^{-2r/a_0}\, dr$$

$$\Rightarrow \quad f_G = \frac{4}{G a_0^3} \int_0^\infty r e^{-2r/a_0} \sin(Gr)\, dr$$

use table of integrals or integrate by parts to get

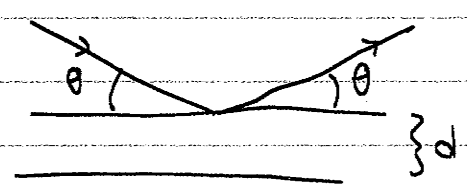
$$f_G = \frac{4}{G a_0^3} \left(\frac{4 a_0^3 G}{(4 + a_0^2 G^2)^2} \right)$$

$$\boxed{f_G = \frac{16}{(4 + a_0^2 G^2)^2}}$$

③ distance between (110) planes is $d^2 = \dfrac{a^2}{h^2+k^2+l^2}$

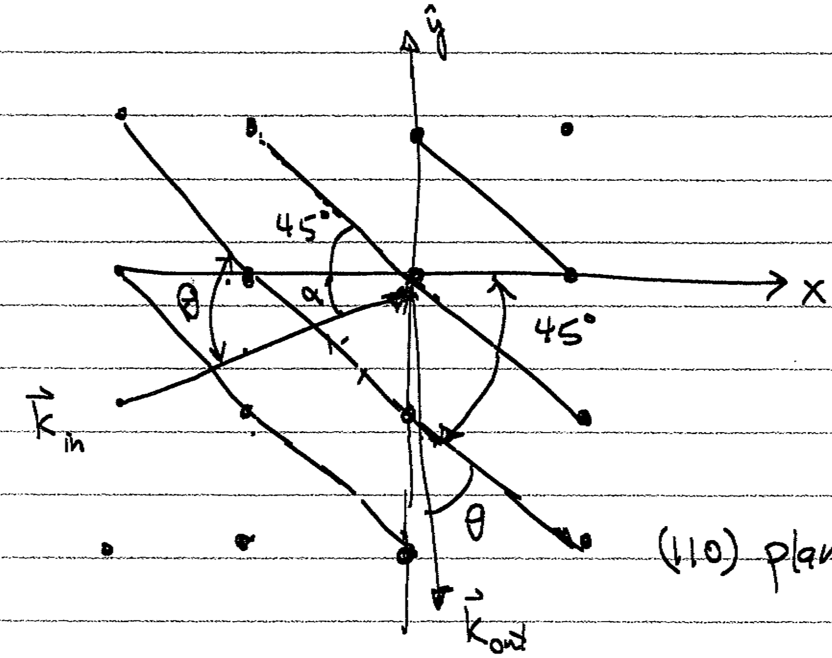
$$\Rightarrow \quad d = \frac{a}{\sqrt{1+1}} = \frac{a}{\sqrt{2}} \qquad a = 3\,\text{Å}$$

Bragg condition:



$$n\lambda = 2d\sin\theta \quad \Rightarrow \quad \lambda = \frac{2d}{n}\sin\theta$$

now, $\vec{k}$ is in [2 1 0] direction, so



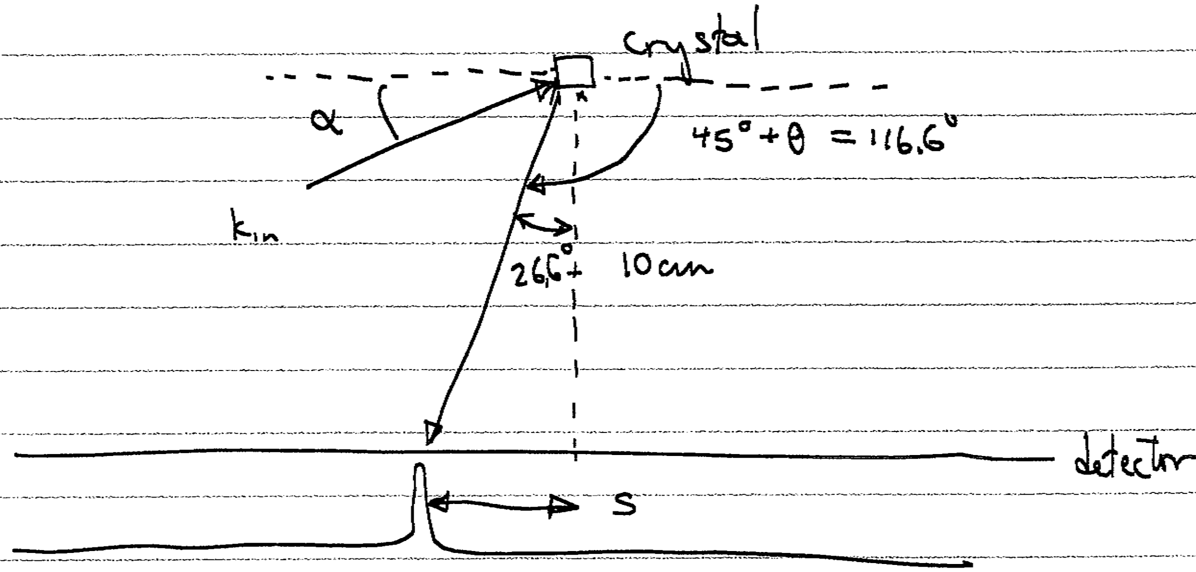
(110) planes

$\tan\alpha = \frac{1}{2}$ so $\alpha = 26.56°$, & $\theta = 45° + 26.56° = 71.6°$

now the min. wavelength corresponds to $n=1$, so we have

$$\lambda = 2d\sin\theta$$
$$= \sqrt{2}\,a\sin\theta \quad (a = 3\text{Å})$$
$$\boxed{= 4.02\ \text{Å}}$$

(b)



$$\tan 26.6° = \frac{S}{10\,\text{cm}} \Rightarrow \boxed{S = 5\text{ cm}}$$