Assignment 4

February 26, 2021

1. Show the Fourier transformation of face centered cubic direct lattice is a body centered lattice in the reciprocal space.

2. (a) Show clearly, with all steps, that the Fourier transformation of a direct lattice is indeed the reciprocal lattice.

   (b) Prove the shift theorem used in Fourier theory, i.e., if in 1D,

$$\mathcal{F}(f(x)) = \hat{F}(k)$$
$$\mathcal{F}(f(x-a)) = \hat{F}(k)e^{-ika}$$

3. Cs and CsCl are both simple primative Bravais lattices. In each case:

   (a) Identify the basis.

   (b) Find the structure factor $S(hkl)$.

   (c) Mention a few planes which give/do not give scattered intensities.

4. Consider the accompanying figure showing scattering of X-rays of wavelength λ from a one-dimensional crystal with monoatomic basis and spacing a. The vector $\vec{s}_o$ and $\vec{s}$ are incident and scattered directions. Note the vector $\vec{a}$ and angle α_o and β_o.

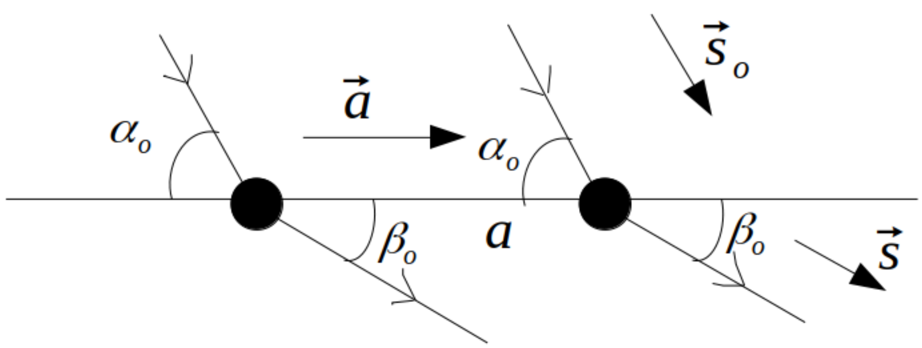

Figure 1

(a) Scattering takes place when the path difference is an integral number of wavelength, $n_x\lambda$. What is the path difference between the two scattered X-rays?

(b) Show that in vectorial form

$$\vec{a}.(\vec{s}-\vec{s_o}) = n_x\lambda \quad (1)$$

(c) Write similar vectorial equations for the x, y, z directions in a 3D crystal, i.e.

$$\vec{b}.(\vec{s}-\vec{s_o}) = n_y\lambda \quad (2)$$

$$\vec{c}.(\vec{s}-\vec{s_o}) = n_z\lambda \quad (3)$$

(d) Show graphically that Eq. 1 results in scattering along the surface of a cone. What is the axis of this cone?

(e) The figure 2 is called the Lane formulation. By the equivalence of Lane and Bragg formulation, show the n_x, n_y and n_z in Eqs. 1-3 are Miller indices of the Miller planes.

5. The length of a reciprocal lattice vector normal to an (hkl) plane is

$$|\vec{d^*_{hkl}}| = \frac{2\pi}{d_{hkl}},$$

where d_{hkl} is the inter planar spacing.

(a) Show that for an orthogonal crystal system

$$\frac{1}{d_{hkl}} = \left(\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}\right)^{\frac{1}{2}} \quad (4)$$

In this part, I require you to use the formula for a vector length and the definition of the reciprocal lattice vectors $(\vec{a^*}, \vec{b^*}, \vec{c^*})$. How does this formula look when we have a cubic crystal system?

(b) Consider an (hkl) plane in an orthogonal system

i. What are the intercepts of the plane along each of the three $\vec{a}$, $\vec{b}$ and $\vec{c}$ axes?

ii. Consider a vector $\vec{p}$ which connects the origin to the plane at right angles. Find the projections of $\vec{p}$ onto the three side planes (ab), (bc) and (ac) of the orthorhombic unit cell. One such projection is shown in figure 3.

iii. Suppose the projection makes angles θ_1, θ_2 and θ_3 with $\vec{a}$, $\vec{b}$ and $\vec{c}$ respectively. The values $cos\theta_1$, $cos\theta_2$ and $cos\theta_3$ are called direction cosines of $\vec{p}$. Using $cos^2\theta_1 + cos^2\theta_2 + cos^2\theta_3 = 1$, derive the length, $|\vec{p}|$ and show it matches the result from part (a).

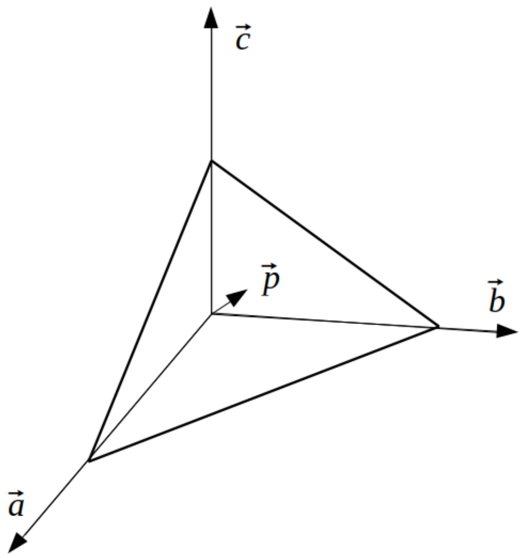

Figure 2

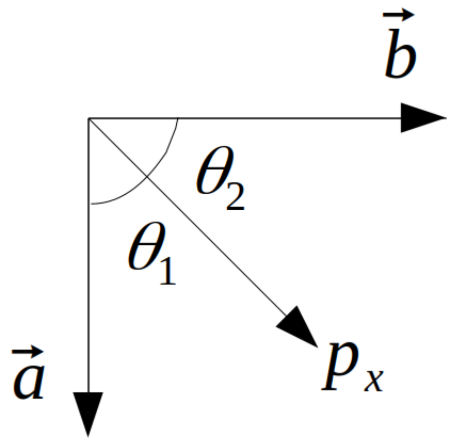

Figure 3

6. $BaTiO_3$ is $Pm\bar{3}m$. The basis is:

$$
\begin{array}{ll}
Ba & [0,0,0] \\
Ti & \left[\frac{1}{2},\frac{1}{2},\frac{1}{2}\right] \\
O & \left[\frac{1}{2},\frac{1}{2},0\right], \left[\frac{1}{2},0,\frac{1}{2}\right], \left[0,\frac{1}{2},\frac{1}{2}\right].
\end{array}
$$

$sin^2\theta$	N	$h\ k\ l$
0.1365		
0.1820		
0.3640		
0.5005		
0.5460		
0.7280		
0.8645		
0.9100		

(a) Sketch the unit cell.

(b) Find $S(001)$ where the atomic form factors are f_{Ba}, f_{Ti}, f_O, i.e. find $S(hkl)$ for $h = 0, k = 0, l = 1$. You are required to find the structure factors for both the lattice and the basis. Then multiply the two together.

7. Copper ($Fm\bar{3}m$) is shone with X-rays ($\lambda = 154pm$).

   (a) Show that for the scattering angle θ,

$$sin^2\theta = \frac{\lambda^2}{4a^2}(h^2 + k^2 + l^2) = \frac{\lambda^2}{4a^2}N = A \times N.$$

   where $N = h^2 + k^2 + l^2$ must be an integer.

   (b) A real experiment yields the scattering directions tabulated in the given table. Complete the table and in the process verify that the crystal system is cubic and find the unit cell size.

8. Find the systematic absences in the diamond $Fd\bar{3}m$ crystal structure.