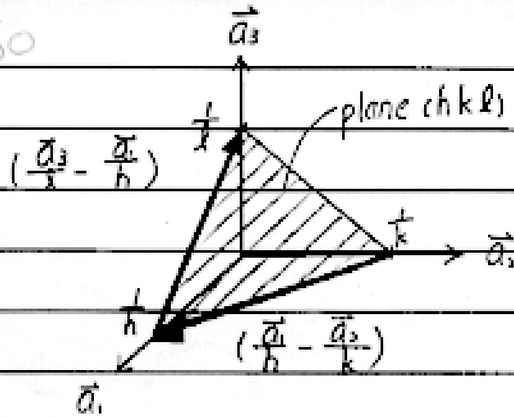
Assignment 2

Total : 60



1(a) Consider any 2 vectors on the plane (hkl).

e.g. $\left(\frac{\vec a_3}{l} - \frac{\vec a_1}{h}\right)$ and $\left(\frac{\vec a_1}{h} - \frac{\vec a_2}{k}\right)$

Then, $\left(\frac{\vec a_3}{l} - \frac{\vec a_1}{h}\right) \cdot \vec G$

$$= \left(\frac{\vec a_3}{l} - \frac{\vec a_1}{h}\right) \cdot (h\vec b_1 + k\vec b_2 + l\vec b_3)$$

$$= \left(\frac{\vec a_3}{l} - \frac{\vec a_1}{h}\right) \cdot \left[2\pi h \frac{\vec a_2 \times \vec a_3}{\vec a_1 \cdot \vec a_2 \times \vec a_3} + 2\pi k \frac{\vec a_3 \times \vec a_1}{\vec a_1 \cdot \vec a_2 \times \vec a_3} + 2\pi l \frac{\vec a_1 \times \vec a_2}{\vec a_1 \cdot \vec a_2 \times \vec a_3}\right]$$

$$= 2\pi \frac{\cancel{\vec a_3 \cdot \vec a_1 \times \vec a_2}}{\cancel{\vec a_1 \cdot \vec a_2 \times \vec a_3}} - 2\pi \frac{\cancel{\vec a_1 \cdot \vec a_2 \times \vec a_3}}{\cancel{\vec a_1 \cdot \vec a_2 \times \vec a_3}}$$

$$= 0$$

and $\left(\frac{\vec a_1}{h} - \frac{\vec a_2}{k}\right) \cdot \vec G$

$$= \left(\frac{\vec a_1}{h} - \frac{\vec a_2}{k}\right) \cdot (h\vec b_1 + k\vec b_2 + l\vec b_3)$$

$$= \left(\frac{\vec a_1}{h} - \frac{\vec a_2}{k}\right) \cdot \left[2\pi h \frac{\vec a_2 \times \vec a_3}{\vec a_1 \cdot \vec a_2 \times \vec a_3} + 2\pi k \frac{\vec a_3 \times \vec a_1}{\vec a_1 \cdot \vec a_2 \times \vec a_3} + 2\pi l \frac{\vec a_1 \times \vec a_2}{\vec a_1 \cdot \vec a_2 \times \vec a_3}\right]$$

$$= 2\pi \frac{\cancel{\vec a_1 \cdot \vec a_2 \times \vec a_3}}{\cancel{\vec a_1 \cdot \vec a_2 \times \vec a_3}} - 2\pi \frac{\cancel{\vec a_2 \cdot \vec a_3 \times \vec a_1}}{\cancel{\vec a_1 \cdot \vec a_2 \times \vec a_3}}$$

$$= 0$$

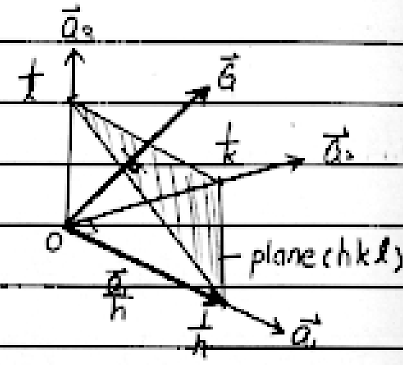
$\therefore$ $\vec G \perp \left(\frac{\vec a_3}{l} - \frac{\vec a_1}{h}\right)$ and $\vec G \perp \left(\frac{\vec a_1}{h} - \frac{\vec a_2}{k}\right)$

$\Rightarrow$ $\vec G \perp$ plane (hkl) #

5

(b) The required distance
= distance between the origin to the plane $(hk\ell)$

Consider a vector pointing to any one point on the plane
e.g. $\frac{\vec{a}_1}{h}$ ①



The required distance $d(hk\ell)$
= the projection of $\frac{\vec{a}_1}{h}$ on unit vector $\hat{G}$

$$= \frac{\vec{a}_1}{h} \cdot \frac{\vec{G}}{|\vec{G}|} \quad ①$$

$$= \frac{\vec{a}_1}{h} \cdot \frac{(h\vec{b}_1 + k\vec{b}_2 + \ell\vec{b}_3)}{|\vec{G}|}$$

$$= \frac{\vec{a}_1 \cdot \vec{b}_1}{|\vec{G}|}$$

$$= \frac{2\pi}{|\vec{G}|} \quad ①$$

3

(c) For SC lattice,

$$\vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3} = 2\pi \frac{a\hat{y} \times a\hat{z}}{a\hat{x} \cdot a\hat{y} \times a\hat{z}} = \frac{2\pi}{a^3}(a^2\hat{x}) = \frac{2\pi}{a}\hat{x} \quad ①$$

$$\vec{b}_2 = 2\pi \frac{\vec{a}_3 \times \vec{a}_1}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3} = 2\pi \frac{a\hat{z} \times a\hat{x}}{a\hat{x} \cdot a\hat{y} \times a\hat{z}} = \frac{2\pi}{a^3}(a^2\hat{y}) = \frac{2\pi}{a}\hat{y} \quad ①$$

$$\vec{b}_3 = 2\pi \frac{\vec{a}_1 \times \vec{a}_2}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3} = 2\pi \frac{a\hat{x} \times a\hat{y}}{a\hat{x} \cdot a\hat{y} \times a\hat{z}} = \frac{2\pi}{a^3}(a^2\hat{z}) = \frac{2\pi}{a}\hat{z} \quad ①$$

$$\therefore \quad \vec{G} = h\left(\frac{2\pi}{a}\hat{x}\right) + k\left(\frac{2\pi}{a}\hat{y}\right) + \ell\left(\frac{2\pi}{a}\hat{z}\right)$$

$$|\vec{G}| = \sqrt{\left(\frac{2\pi}{a}h\right)^2 + \left(\frac{2\pi}{a}k\right)^2 + \left(\frac{2\pi}{a}\ell\right)^2}$$

$$= \frac{2\pi}{a}\sqrt{h^2 + k^2 + \ell^2} \quad ①$$

$$d^2 = \frac{(2\pi)^2}{|\vec{G}|^2}$$

$$= \frac{a^2}{h^2 + k^2 + \ell^2} \quad ①$$

5

2). $V_{Brillouin} = \vec{b}_1 \cdot \vec{b}_2 \times \vec{b}_3$ (1)

$$= (2\pi)^3 \left[\frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3} \cdot \frac{\vec{a}_3 \times \vec{a}_1}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3} \times \frac{\vec{a}_1 \times \vec{a}_2}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3} \right]$$ (1)

$$= (2\pi)^3 \left[\frac{\vec{a}_2 \times \vec{a}_3 \cdot \cancel{(-\vec{a}_3 \cdot \vec{a}_1 \times \vec{a}_2)}\vec{a}_1}{(\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3)^{\cancel{3}\,2}} \right]$$ (by vector identity)

$$= (2\pi)^3 \left[\frac{\cancel{\vec{a}_2 \times \vec{a}_3 \cdot \vec{a}_1}}{(\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3)^2} \right]$$

$$= \frac{(2\pi)^3}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3}$$

$$= \frac{(2\pi)^3}{V_c}$$ // (1)

3

3) The reciprocal lattice vectors are:

$$\vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3} = \frac{2\pi\, b\hat{y} \times c\hat{z}}{a\hat{x} \cdot b\hat{y} \times c\hat{z}} = 2\pi \frac{bc\,\hat{x}}{abc} = 2\pi \frac{\hat{x}}{a}$$ (1)

$$\vec{b}_2 = 2\pi \frac{\vec{a}_3 \times \vec{a}_1}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3} = \frac{2\pi\, c\hat{z} \times a\hat{x}}{a\hat{x} \cdot b\hat{y} \times c\hat{z}} = 2\pi \frac{ca\,\hat{y}}{abc} = 2\pi \frac{\hat{y}}{b}$$ (1)

$$\vec{b}_3 = 2\pi \frac{\vec{a}_1 \times \vec{a}_2}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3} = \frac{2\pi\, a\hat{x} \times b\hat{y}}{a\hat{x} \cdot b\hat{y} \times c\hat{z}} = 2\pi \frac{ab\,\hat{z}}{abc} = 2\pi \frac{\hat{z}}{c}$$ // (1)

$$\therefore \quad \vec{G} = h\left(\frac{2\pi}{a}\hat{x}\right) + k\left(\frac{2\pi}{b}\hat{y}\right) + l\left(\frac{2\pi}{c}\hat{z}\right)$$

$$|\vec{G}| = 2\pi \sqrt{\left(\frac{h}{a}\right)^2 + \left(\frac{k}{b}\right)^2 + \left(\frac{l}{c}\right)^2}$$

$$d = \frac{2\pi}{|\vec{G}|}$$

$$= \frac{1}{\sqrt{\left(\frac{h}{a}\right)^2 + \left(\frac{k}{b}\right)^2 + \left(\frac{l}{c}\right)^2}}$$ // (1)

$$d(100) = \left[\left(\frac{1}{3.17 \times 10^{-10}}\right)^2 + \left(\frac{0}{4.85 \times 10^{-10}}\right)^2 + \left(\frac{0}{2.13 \times 10^{-10}}\right)^2 \right]^{-1/2} = 3.17\,\text{Å}$$ // (1)

$$d(110) = \left[\left(\frac{1}{3.17 \times 10^{-10}}\right)^2 + \left(\frac{1}{4.85 \times 10^{-10}}\right)^2 \right]^{-1/2} = 2.65\,\text{Å}$$ // (1)

$$d(111) = \left[\left(\frac{1}{3.17 \times 10^{-10}}\right)^2 + \left(\frac{1}{4.85 \times 10^{-10}}\right)^2 + \left(\frac{1}{2.13 \times 10^{-10}}\right)^2 \right]^{-1/2} = 1.66\,\text{Å}$$ // (1)

4). $\Delta\vec{k} = \vec{G}$ [condition for intensity peak occurs]

$$\vec{k}' - \vec{k} = \vec{G}$$

$$\vec{k}' = \vec{G} + \vec{k}$$

$$\cancel{|\vec{k}'|^2} = (\vec{G} + \vec{k})^2$$

$$= |\vec{G}|^2 + 2\vec{k}\cdot\vec{G} + \cancel{|\vec{k}|^2}$$ (1) [$\because$ $|\vec{k}| = |\vec{k}'|$ for elastic scattering]

$$-2\vec{k}\cdot\vec{G} = |\vec{G}|^2$$

$$\vec{k}\cdot\vec{G} = -\frac{1}{2}|\vec{G}|^2$$ (1)

2

5 (a) For SC,

$$d(hkl) = \frac{a}{\sqrt{h^2+k^2+l^2}}$$ [from Q1 (c)]

then,

$$2d(hkl)\sin\theta = n\lambda$$

$$\lambda = \frac{2a\sin\theta}{\sqrt{h^2+k^2+l^2}}$$ (1) [for $n = 1$]

$$\therefore \lambda_{(100)} = \frac{2\times 4.5\times10^{-10}\sin\left(\frac{40^\circ}{2}\right)}{\sqrt{1^2+0^2+0^2}}$$

$$= 3.08\ \text{Å}$$ (1)

$$\lambda_{(110)} = \frac{2\times 4.5\times10^{-10}\sin\left(\frac{40^\circ}{2}\right)}{\sqrt{1^2+1^2+0^2}}$$

$$= 2.18\ \text{Å}$$ (1)

$$\lambda_{(110)} = \frac{2\times 4.5\times10^{-10}\sin\left(\frac{40^\circ}{2}\right)}{\sqrt{1^2+1^2+1^2}}$$

$$= 1.78\ \text{Å}$$ (1)

4

(b)
$$\sin\theta = \frac{\lambda}{2d}$$

$$= \frac{\lambda\sqrt{h^2+k^2+l^2}}{2a}$$ (1)

$$2\theta_{(100)} = 2\sin^{-1}\frac{2.18\times10^{-10}\sqrt{1^2+0^2+0^2}}{2\times4.5\times10^{-10}}$$

3

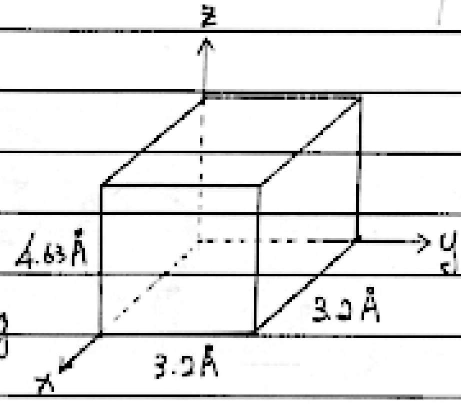
$$= 28^\circ$$ (1)

$$2\theta_{(111)} = 2\sin^{-1}\frac{2.18\times10^{-10}\sqrt{3}}{2\times4.5\times10^{-10}}$$

$$= 49.6^\circ$$

5(c) $2\theta_{(220)} = 2\sin^{-1}\dfrac{2.18\times10^{-10}\sqrt{2^2+2^2}}{2\times4.5\times10^{-10}}$

$= 86.5°$ ※



6(a) By Bragg law,

$2d\sin\theta = n\lambda$

$\sin\theta = \dfrac{n\lambda}{2d}$

Smallest θ gives smallest diameter ring

For smallest θ, $n=1$

and d is the largest separation.

From Q1(b), $d \propto \dfrac{1}{\text{plane indices}}$

$\Rightarrow$ consider the plane with the smallest indices, i.e. (100), (010), (001)

In (100), $d = 3.2$ Å

In (010), $d = 3.2$ Å

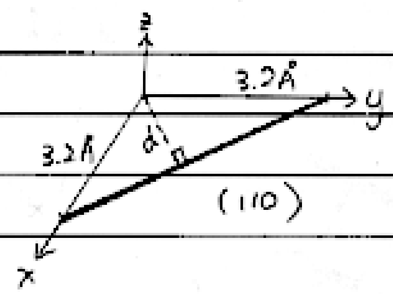
In (001), $d = 4.63$ Å

$\Rightarrow$ consider the plane with the 2nd smallest indices,

i.e. (110), (011), (101)

In (110), $d = \frac{1}{2}\sqrt{3.2^2+3.2^2}$ Å

$= 2.26$ Å

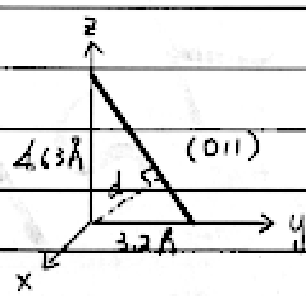


In (011), $d = 4.63\times3.2/\sqrt{4.63^2+3.2^2}$

$= 2.63$ Å

In (101), $d = 4.63\times3.2/\sqrt{4.63^2+3.2^2}$

$= 2.63$ Å

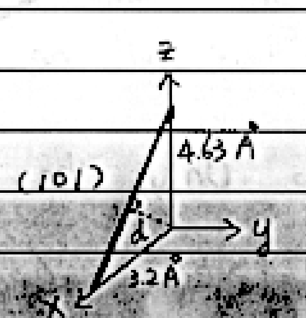


$\therefore$ the 3 largest d are

$d_1 = 4.63$ Å

$d_2 = 3.2$ Å

$d_3 = 2.63$ Å



$\therefore$ smallest θ are

$$\theta_1 = \sin^{-1} \frac{1.54\,Å}{2 \times 4.63\,Å}$$

$$= 9.57^\circ$$

$$\theta_2 = \sin^{-1} \frac{1.54\,Å}{2 \times 3.2\,Å}$$

$$= 13.92^\circ$$

$$\theta_3 = \sin^{-1} \frac{1.54\,Å}{2 \times 2.63\,Å}$$

$$= 17.02^\circ$$

$\therefore$ The forward scattering angles are $2\theta_1$, $2\theta_2$, $2\theta_3$

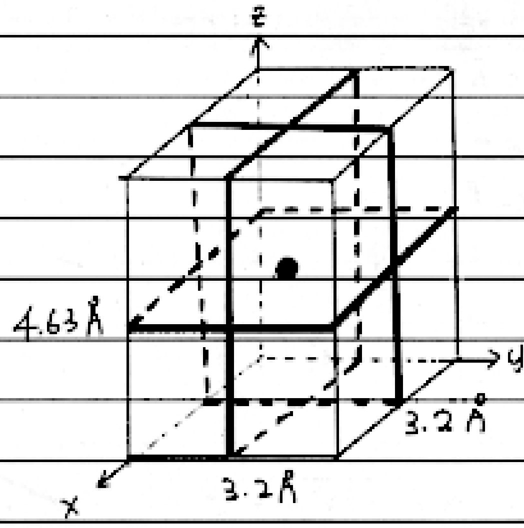
$= 19.2^\circ, 27.9^\circ, 34.0^\circ$ #

3

The backscattering angles (please go to the last page!)

8

(b)



3

If there is a different atom at the center, there will be an extra plane in (100), (010) and (001). 1

thus, d_1 and d_2 will be decreased and the scattering intensity in θ_1 and θ_2 will also be decreased.

$\because$ the center atom is on the plane (110) (101) and (011) 1

$\therefore$ there will be no extra planes and d_3 will not be changed

1

$\therefore$ Only the 2 smallest diameter rings will be weakened #

7(a) $\theta_1 = \frac{24.4^\circ}{2}$, $\sin^2\theta_1 = 0.0447$

$\theta_2 = \frac{28.2^\circ}{2}$, $\sin^2\theta_2 = 0.0593$

$\theta_3 = \frac{40.3^\circ}{2}$, $\sin^2\theta_3 = 0.1187$

$\theta_4 = \frac{47.7^\circ}{2}$, $\sin^2\theta_4 = 0.1635$

$\theta_5 = \frac{50^\circ}{2}$, $\sin^2\theta_5 = 0.1786$. * 5

$$\frac{\sin^2\theta_1}{\sin^2\theta_2} = \frac{0.0447}{0.0593} = 0.7538$$ 1

By Bragg law, $2d\sin\theta = \lambda$ [take $n=1$]

$$\sin^2\theta = \left(\frac{\lambda}{2}\right)^2 \frac{1}{d^2}$$

$$\therefore \frac{\sin^2\theta_1}{\sin^2\theta_2} = \frac{d_2^2}{d_1^2}$$

*[Note that : $\theta_1, \theta_2, \theta_3 \ldots$ are the smallest angles, $(\sin^2\theta \propto \frac{1}{d^2})$

$\Rightarrow d_1, d_2, d_3 \ldots$ are the largest plane separations.

$\because d \propto \frac{1}{\text{plane indice}}$

$\therefore$ To obtain the largest d, we consider the smallest plane indice, i.e. (100), (010), (001); (110), (011), (101); ...]

For SC, $d^2 = \frac{(2\pi)^2}{|G|^2} = \frac{a^2}{h^2+k^2+l^2}$ 1

$$d_1^2 = \frac{a^2}{1+0+0} = \frac{a^2}{0+1+0} = \frac{a^2}{0+0+1} = a^2$$

$$d_2^2 = \frac{a^2}{1+1+0} = \frac{a^2}{1+0+1} = \frac{a^2}{0+0+1} = a^2/2$$

$$\Rightarrow \frac{d_2^2}{d_1^2} = \frac{1}{2} \neq 0.7538$$ 1

$\therefore$ it is not a SC lattice.

For BCC, $d^2 = \frac{(2\pi)^2}{|G|^2} = \frac{a^2}{(k+l)^2+(h+l)^2+(h+k)^2}$ 1

$$d_1^2 = \frac{a^2}{0+1+1} = \frac{a^2}{1+0+1} = \frac{a^2}{1+1+0} = \frac{a^2}{2}$$

$$d_2^2 = \frac{a^2}{1+1+4} = \frac{a^2}{1+4+1} = \frac{a^2}{4+1+1} = \frac{a^2}{6}$$

$$\Rightarrow \frac{d_2^2}{d_1^2} = \frac{1}{3} \neq 0.7538$$ 1

$\therefore$ it is not a BCC lattice.

For FCC, $d^2 = \frac{(2\pi)^2}{|G|^2}$

$$= \frac{a^2}{(-h+k+\ell)^2 + (h-k+\ell)^2 + (h+k-\ell)^2} \quad 1$$

$$d_1^2 = \frac{a^2}{1+1+1} = \frac{a^2}{3}$$

$$d_2^2 = \frac{a^2}{0+0+4} = \frac{a^2}{0+4+0} = \frac{a^2}{4+0+0} = \frac{a^2}{4}$$

$$\Rightarrow \frac{d_2^2}{d_1^2} = \frac{3}{4} \quad \cancel{\approx 0.7538} \quad 1$$

$\therefore$ it is a FCC lattice # 1 13

7(b) $\sin^2\theta_1 = \left(\frac{\lambda}{2}\right)^2 \frac{1}{d_1^2}$ 1

$$0.0447 = \left(\frac{1.39\,Å}{2}\right)^2 \frac{3}{a^2} \quad 1$$

$$a = 5.7\,Å \;\# \quad 1$$

3

7(c) For FCC, $\vec{G} = h\vec{b}_1 + k\vec{b}_2 + \ell\vec{b}_3$ [in reciprocal lattice space]

$$= \frac{2\pi}{a}[(-h+k+\ell)\hat{x} + (h-k+\ell)\hat{y} + (h+k-\ell)\hat{z}]$$

$$= \frac{2\pi}{a}(p\hat{x} + q\hat{y} + r\hat{z}) \quad \text{[in } \hat{x}\hat{y}\hat{z} \text{ space]}$$

where $\begin{cases} p = -h+k+\ell \\ q = h-k+\ell \\ r = h+k-\ell \end{cases}$; h, k, l must be integers $\Rightarrow$ p, q, r are integers

$$\Rightarrow |\vec{G}| = \frac{2\pi}{a}\sqrt{p^2+q^2+r^2}$$

By Bragg law, $2d\sin\theta = \lambda$ (take $n=1$)

$$\frac{2}{\lambda}\sin\theta = \frac{1}{d}$$

$$\frac{1}{d^2} = \left(\frac{2}{\lambda}\right)^2 \sin^2\theta$$

$$p^2+q^2+r^2 = \left(\frac{2a}{\lambda}\right)^2 \sin^2\theta \qquad \left[\frac{1}{d^2} = \frac{|G|^2}{(2\pi)^2}\right]$$

$$= \left(\frac{2 \times 5.69\,Å}{1.39\,Å}\right)^2 \sin^2\theta$$

$\theta_1 = \frac{24.4}{2}$, $p^2+q^2+r^2 = 3 \Rightarrow p = q = r = 1$

$\Rightarrow$ the plane indice in the real space xyz = (1 1 1) #

$\theta_2 = \frac{28.2}{2}$, $p^2+q^2+r^2 = 4$

$\Rightarrow$ (200), (020) or (002) #

$\theta_3 = \frac{40.3}{2}$, $p^2+q^2+r^2 = 8$

$\Rightarrow$ (220), (202) or (022) #

$\theta_4 = \frac{47.7}{2}$, $p^2+q^2+r^2 = 11$

$\Rightarrow (113), (131)$ or (311) ※

$\theta_5 = \frac{50.0}{2}$ $p^2+q^2+r^2 = 12$

$\Rightarrow (222)$ ※

$\theta_6 = \frac{172.8}{2}$, $p^2+q^2+r^2 = 67$

$\Rightarrow (733), (373)$ or (337) ※

$\theta_7 = \frac{154.6}{2}$ $p^2+q^2+r^2 = 64$

$\Rightarrow (800), (080)$ or (008) ※

$\theta_8 = \frac{139}{2}$, $p^2+q^2+r^2 = 59$

$\Rightarrow (553), (535)$ or (355) ※

$\theta_9 = \frac{131.7}{2}$ $p^2+q^2+r^2 = 56$

$\Rightarrow (642), (624), (426), (462), (246)$ or (264) ※

$\theta_{10} = \frac{123.1}{2}$ $p^2+q^2+r^2 = 52$

$\Rightarrow (640), (604), (406), (460), (046)$ or (064) ※

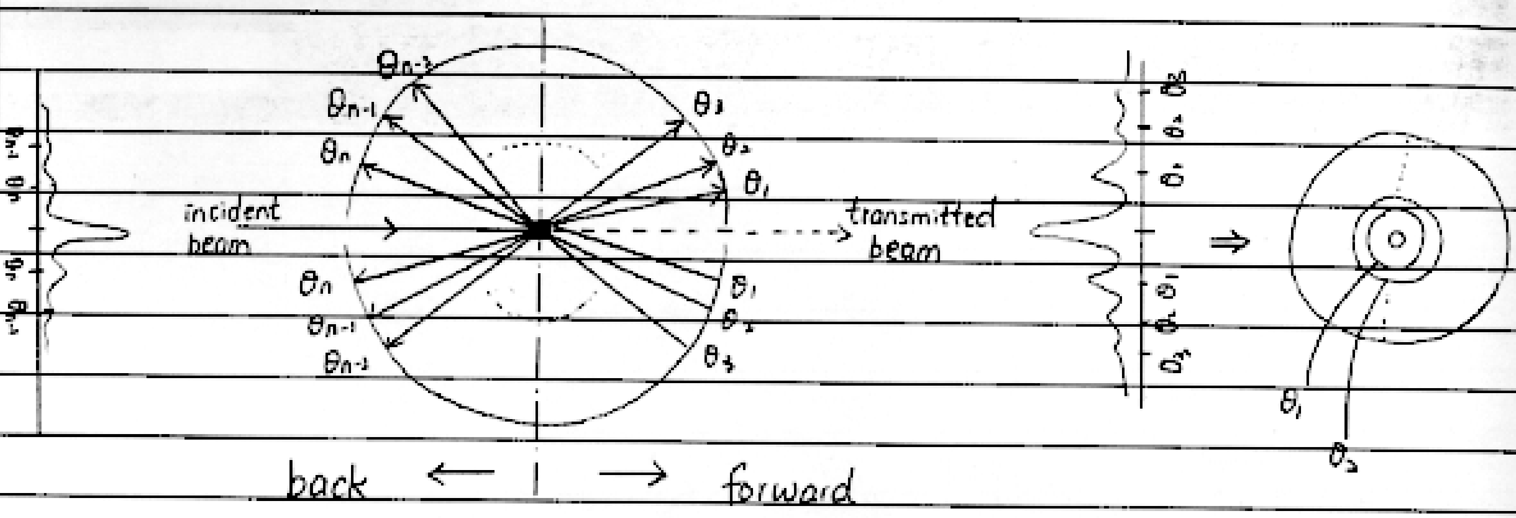
※ [Note: From the above results, we can see that the indices in real space for FCC lattice – 'p, q, r' must be all even integers or all odd integer. This can be proved by the structure factor. (Text book p. 45 - 49)]

(d). $\sin^2\theta_6 = \left(\frac{\lambda}{2}\right)^2 \frac{1}{d^2}$

$$\sin^2\left(\frac{172.8}{2}\right) = \left(\frac{1.39\,\text{Å}}{2}\right)^2 \frac{67}{a^2}$$

$a = 5.7\,\text{Å}$ ※

6(a) <u>Back scattering angle</u>



θ : scattered angle

Forward scattering $\Rightarrow$ $0 \leq \theta \leq 90°$
Back scattering $\Rightarrow$ $90° \leq \theta \leq 180°$

$$2d \sin\theta = n\lambda$$

$$\sin\frac{\theta_n}{2} = \frac{n\lambda}{2d}$$

$$\sin\frac{\theta_n}{2} = \frac{1.54}{2d} \quad \text{(take } n=1\text{)}$$

By calculating d in the other planes, θ_n, θ_{n-1} and θ_{n-2} can be found. However, the crystal lattice is not a cubic. Thus, we have to find d by trials. (It is too time-consuming, you can have a try if you have time ^v^b. Good luck!)