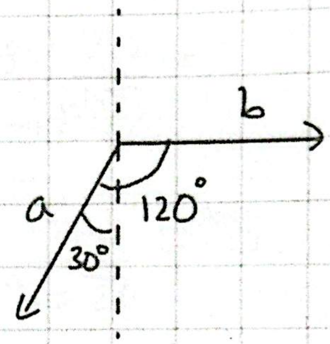
Assignment 3

Solution

Question 1:-

a) Because this is a hexagonal lattice, the angle b/w $\vec{a}$ and $\vec{b}$ is $120°$.



$$\Rightarrow \quad \vec{b} = b\hat{j} \quad ; \quad \Rightarrow \quad \vec{c} = c\hat{k}$$

$$\Rightarrow \quad \vec{a} = b\left[\cos(30°)\hat{i} - \sin(30°)\hat{j}\right]$$

$$= b\left[\frac{\sqrt{3}}{2}\hat{i} - \frac{1}{2}\hat{j}\right]$$

b) The reciprocal lattice vectors are:-

$$\vec{a}^* = 2\pi \frac{\vec{b}\times\vec{c}}{\vec{a}\cdot(\vec{b}\times\vec{c})} \quad ; \quad \vec{b}^* = 2\pi \frac{\vec{c}\times\vec{a}}{\vec{a}\cdot(\vec{b}\times\vec{c})} \quad ;$$

$$\vec{c}^* = 2\pi \frac{\vec{a}\times\vec{b}}{\vec{a}\cdot(\vec{b}\times\vec{c})}$$

$$\Rightarrow \vec{a}\cdot(\vec{b}\times\vec{c}) = \vec{a}\cdot\left(\begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ 0 & b & 0 \\ 0 & 0 & c \end{vmatrix}\right) = \vec{a}\cdot\left(bc\hat{i}\right)$$

$$= \frac{\sqrt{3}}{2} c b^2$$

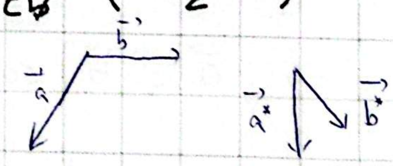
$$\vec{a}^* = \frac{2\pi(2)}{\sqrt{3}\,\cancel{c}b^2}\left(b\cancel{c}\right)\hat{\imath} = \frac{4\pi}{\sqrt{3}\,b}\hat{\imath}$$

$$\vec{b}^* = \frac{2\pi(2)}{\sqrt{3}\,cb^2}\begin{vmatrix} \hat{\imath} & \hat{\jmath} & \hat{k} \\ 0 & 0 & c \\ \sqrt{3}/2\, b & -1/2\, b & 0 \end{vmatrix} = -cb\left(-\frac{1}{2}\hat{\imath} - \frac{\sqrt{3}}{2}\hat{\jmath}\right)\frac{4\pi}{\sqrt{3}\,cb^2}$$

$$= \frac{2\pi}{\sqrt{3}\,b}\left(\hat{\imath} + \sqrt{3}\,\hat{\jmath}\right)$$

$$\vec{c}^* = \frac{4\pi}{\sqrt{3}\,cb^2}\begin{vmatrix} \hat{\imath} & \hat{\jmath} & \hat{k} \\ b\sqrt{3}/2 & -b/2 & 0 \\ 0 & b & 0 \end{vmatrix} = -\frac{\overset{2}{\cancel{4}}\pi\,\cancel{b^2}}{\cancel{\sqrt{3}}\,c\cancel{b^2}}\left(-\frac{\cancel{\sqrt{3}}}{\cancel{2}}\hat{k}\right)$$

$$= \frac{2\pi}{c}\hat{k}$$



See orientations here.

c) For a lattice with a basis of two identical atoms:

$$(0,0,0) \quad , \quad (2/3, 1/3, 1/2)$$

$$\Rightarrow S_{hkl}^{(basis)} = \sum_n f_n \exp\left[2\pi i\left(hx_n + ky_n + lz_n\right)\right]$$

$$= f e^{2\pi i(0)} + f\exp\left[2\pi i\left(\frac{2}{3}h + \frac{1}{3}k + \frac{1}{2}l\right)\right]$$

$$= f\left(1 + \exp\left[\frac{2\pi i}{3}(2h+k)\right]e^{i\pi l}\right)$$

d) $$S_{hkl}^{(overall)} = S_{hkl}^{(lattice)}\,S_{hkl}^{(basis)}$$

For a primitive lattice, $S_{hkl}^{(lattice)} = 1$ (no extra centering phase factor)

$$\therefore \quad S_{hkl}^{(overall)} = S_{hkl}^{(basis)}$$
$$= f\left(1 + \exp\left[\frac{2\pi i}{3}(2h+k)\right]e^{i\pi l}\right)$$

$$S_{hkl}^{(overall)} = S = f\left(1 + (-1)^l \underbrace{\exp\left[\frac{2\pi i}{3}(2h+k)\right]}\right)$$

This results in three cases:-
$m = 2h+k \pmod 3$
$= 0, 1, 2$

where f is the atomic scattering factor for the atom.

$$\Rightarrow m = 0 \quad ; \quad S = f\left[1 + (-1)^l\right]$$
$$= \begin{cases} 2f & l = 2n \\ 0 & l = 2n-1 \end{cases}$$
$$\therefore I \propto |S|^2 = \begin{cases} 4f^2 & l = 2n \\ 0 & l = 2n-1 \end{cases}$$

$$\Rightarrow m = 1 \quad ; \quad S = f\left[1 + (-1)^l e^{2\pi i/3}\right]$$
$$= \begin{cases} 1 + e^{2\pi i/3} & l = 2n \\ 1 - e^{2\pi i/3} & l = 2n-1 \end{cases}$$
$$\therefore I \propto |S|^2 = \begin{cases} \left(1 + e^{2\pi i/3}\right)\left(1 + e^{-2\pi i/3}\right) f^2 & l = 2n \\ \left(1 - e^{2\pi i/3}\right)\left(1 - e^{-2\pi i/3}\right) f^2 & l = 2n-1 \end{cases}$$
$$= \begin{cases} f^2 & l = 2n \\ 3f^2 & l = 2n-1 \end{cases}$$

CamScanner

$$\Rightarrow m = 2 \quad ; \quad S = f\left[1 + (-1)^{\ell} e^{4\pi i/3}\right]$$

$$= \begin{cases} 1 + e^{4\pi i/3} & \ell = 2n \\ 1 - e^{4\pi i/3} & \ell = 2n-1 \end{cases}$$

$$\therefore \; I \propto |S|^2 = \begin{cases} \left(1 + e^{4\pi i/3}\right)\left(1 + e^{-4\pi i/3}\right) f^2 & \ell = 2n \\ \left(1 - e^{4\pi i/3}\right)\left(1 - e^{-4\pi i/3}\right) f^2 & \ell = 2n-1 \end{cases}$$

$$= \begin{cases} f^2 & \ell = 2n \\ 3f^2 & \ell = 2n-1 \end{cases}$$

$\therefore$ The possible intensity

$$I \propto \{0, f^2, 3f^2, 4f^2\}$$

with relative magnitude of non-zero intensities:- 1 : 3 : 4

✓

estion 2:-

$$d_{hkl} = \frac{a}{\sqrt{h^2+k^2+l^2}} \quad ; \quad a = 0.2866 nm$$

For a BCC structure, reflections are only allowed when : $h+k+l = 2n$ (even)

Allowed family of planes:-

- $\{110\}$: $h^2+k^2+l^2 = 2$ $\quad d_{110} = \frac{a}{\sqrt{2}} = 0.2027 nm$
- $\{200\}$: $h^2+k^2+l^2 = 4$ $\quad d_{200} = \frac{a}{2} = 0.1433 nm$
- $\{211\}$: $h^2+k^2+l^2 = 6$ $\quad d_{211} = \frac{a}{\sqrt{6}} = 0.1170 nm$
- $\{220\}$: $h^2+k^2+l^2 = 8$ $\quad d_{220} = \frac{a}{4} = 0.1013 nm$
- $\{310\}$: $h^2+k^2+l^2 = 10$ $\quad d_{310} = \frac{a}{\sqrt{10}} = 0.0906 nm$

b) Bragg's Law : $n\lambda = 2d\sin\theta$

For $n=1$; $\lambda = 2d\sin\theta$, where $\lambda = 0.154 nm$

$$\Rightarrow \theta_{hkl} = \sin^{-1}\left(\frac{\lambda}{2d_{hkl}}\right)$$

{hkl}	θ_{hkl}
{110}	22.3°
{200}	32.5°
{211}	41.1°
{220}	49.5°
{310}	58.1°

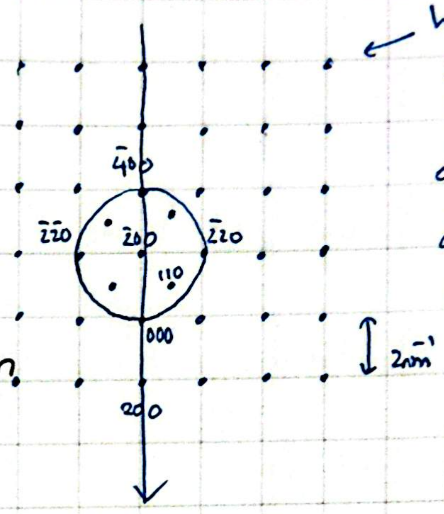
...stion 3:-

Draw an Ewald circle along each of hk0, hk1, hk$\bar{1}$, hk2, hk$\bar{2}$ net.

Reflecting families:-

$$\sin\theta < \frac{\lambda}{2d_{hkl}} \leq 1$$

$$\Rightarrow d_{hkl} \geq \frac{\lambda}{2} = 0.125\,nm$$



Scale
1 box = 2π

$a = 0.5 = \frac{1}{2}$

$a^* = \frac{1}{1/2} = 2$ (in units of 2π)

$\lambda = \frac{1}{4}$

$\frac{1}{\lambda} = 4$

$$\Rightarrow \frac{a}{\sqrt{h^2+k^2+l^2}} \geq 0.125$$

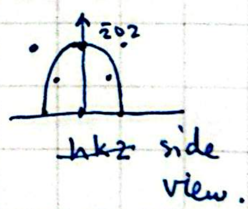
Ewald circle intersects at $(\bar{2}20), (\bar{4}00), (\bar{2}\bar{2}0)$ planes with reflecting directions $[\bar{1}10], [\bar{1}00], [\bar{1}\bar{1}0]$.

Draw a circle of $4\,nm^{-1}$ diameter.

$$\Rightarrow h^2+k^2+l^2 \leq 16$$

$\Rightarrow$ h+k+l must also be even because the structure is BCC.

- For hk1 net, no reflecting plane
- For hk2 net, $(\bar{2}02)$ plane with direction [001].



~~The reflecting plane families are:~~

~~$\{110\}, \{200\}, \{211\}, \{220\}, \{310\}, \{222\}, \{321\}, \{400\}$~~

~~And their corresponding reflecting directions are:-~~

~~$\langle 110\rangle, \langle 100\rangle, \langle 211\rangle, \langle 110\rangle, \langle 310\rangle, \langle 111\rangle, \langle 321\rangle, \langle 100\rangle$~~

$\boxed{\text{This is incorrect}}$

As $d_{hkl} = \frac{0.5}{\sqrt{h^2+k^2+l^2}}$ and $\theta = \sin^{-1}\left(\frac{0.25}{2d_{hkl}}\right)$

$$\Rightarrow \frac{0.5}{\sqrt{h^2+k^2}} \geq 0.125$$

$$\therefore h^2+k^2 = 16$$

For a BCC lattice,

$h+k+l = h+k = 2n$ (even) for reflections

As a result, the allowed family of planes are:-

$\{110\}, \{200\}, \{220\}, \{310\}, \{400\}$,

whose reflecting directions are:

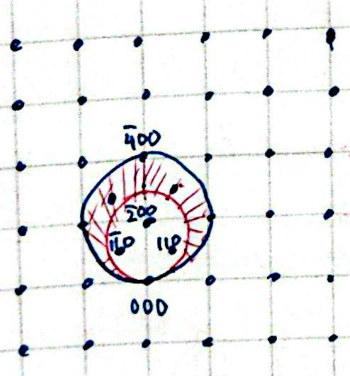
$\langle 110\rangle, \langle 100\rangle, \langle 110\rangle, \langle 310\rangle, \langle 100\rangle$

(b) For part (b), I expect you to draw Ewald circles and solve this problem. For example here is how to find the solution for the hk0 net.

Range of λ is $\frac{1}{4} \longleftrightarrow \frac{3}{10}$ nm.

Range of $1/\lambda$ is $4 \longleftrightarrow \frac{10}{3}$ nm^{-1}.

$= 3.33$ nm^{-1}.



Draw two circles of diameter 4 nm^{-1} and 3.33 nm^{-1} with both circles passing through 000.

Then see the points which are included in the region inbetween the two Ewald circles. These points will indicate the reflecting planes.

Question 4:-

At 4f, the coordinates are :

$$(x,y,\bar{z}),\ (\bar{x},\bar{y},z+\tfrac{1}{2}),\ (\bar{x},\bar{y},\bar{z}),\ (x,y,\bar{z}+\tfrac{1}{2})$$

$$F_{hkl} = f \sum_{j=1}^{4} e^{2\pi i(hx_j + ky_j + lz_j)}$$

for $h = k = 0$ (which is true for $00l$ reflection)

$$F_{00l} = \cancel{f} \sum_{j=1}^{4} e^{2\pi i l z_j}$$

$$= \cancel{f}\left[e^{2\pi i z l} + e^{2\pi i l(z+1/2)} + e^{-2\pi i l z} + e^{-2\pi i l(z-1/2)}\right]$$

$$= \cancel{f}\left[e^{2\pi i z l}\left(1+e^{i\pi l}\right) + e^{-2\pi i l z}\left(1+e^{i\pi l}\right)\right]$$

$$= \cancel{f}\left(1+e^{i\pi l}\right)\frac{\left(e^{2\pi i z l} + e^{-2\pi i l z}\right)}{2}\, 2$$

$$= 2f\left[1+(-1)^l\right]\cos(2\pi z l)$$

$$= \begin{cases} \cancel{4}f\cos(2\pi z l) & l = 2n \ \text{(even)} \\ 0 & l = 2n-1 \ \text{(odd)}. \end{cases}$$

This is the reflection condition mentioned for the 4f Wyckoff positions in the extreme right column.

stion 5:-

Bragg's Law: $2d\sin\theta = n\lambda$

$n=1$; $2d\sin\theta = \lambda$

$\Rightarrow \sin^2\theta \propto \frac{1}{d^2} = \frac{a^2}{\sqrt{h^2+k^2+l^2}}$

This means that the $\sin^2\theta$ values must be proportional to each other

$\Rightarrow$

0.0700/0.0700	=	1.00
0.0763/0.0700	=	1.09
0.1400/0.0700	=	2.00
0.1463/0.0700	=	2.09
0.2163/0.0700	=	3.09
0.2763/0.0700	=	3.95
0.2800/0.0700	=	4.00
0.2863/0.0700	=	4.09
0.3500/0.0700	=	5.00
0.3563/0.0700	=	5.95

— shifted by 0.09, and are not compatible with single parameter a

b) $\sin^2\theta = \frac{\lambda^2}{4d^2} = \frac{\lambda^2}{4}\left[\frac{h^2+k^2}{a^2} + \frac{l^2}{c^2}\right]$

$$= \underbrace{(h^2+k^2)}_{N}\underbrace{\frac{\lambda^2}{4a^2}}_{A} + \underbrace{l^2}_{M}\underbrace{\frac{\lambda^2}{4c^2}}_{B}$$

✓

Allowed values for $N = 0^2+0^2 = 0$

$= 0^2+1^2 = 1$

$= 1^2+1^2 = 2$

$\rightarrow$ 4, 5, 8, 9, 10, 13, ...

[3, 6, 7, ... are not present because these

cannot be decompo[sed]
as h^2+k^2]

Allowed values for $M = 0, 1, 4, 9, 16, 25, \ldots$
(perfect squares) ✓

c) From the data, there are small increment b/w subsequent entries: $0.0763 - 0.0700 = 0.0063$
$0.1463 - 0.1400 = 0.0063$
$\vdots$

And most of the entries are multiples of 0.0700:

$0.0700(1) = 0.0700$
$0.0700(2) = 0.1400$ ✗
$0.0700(4) = 0.2800$
$\vdots$

$\therefore$ $A = 0.0700$, $B = 0.0063$

$\Rightarrow$ $\Rightarrow$ $\sin^2\theta = 0.0700N + 0.0063M$

I have put the complete soluti[on] of (c) in the form of an Excel sheet. In this table $Q = \sin^2\theta$, and we choose a consistent A and B across all entries of $\sin^2\theta$.

Q	A	N	Q-AN	B	M	AN+BM	h	k	l
0.07	0.0175	4	0			0.07	1	0	0
0.0763	0.0175	1	0.0588	0.0588	1	0.0763	0	0	1
0.14	0.0175	8	0	0.0588		0.14	2	2	0
0.1463	0.0175	5	0.0588	0.0588	1	0.1463			
0.2163	0.0175	9	0.0588	0.0588	1	0.2163			
0.2702	0.0175	2	0.2352	0.0588	4	0.2702			
0.28	0.0175	16	0	0.0588		0.28	4	0	0
0.2863	0.0175	13	0.0588	0.0588	1	0.2863			
0.35	0.0175	20	0	0.0588		0.35	4	2	0
0.3563	0.0175	17	0.0588	0.0588	1	0.3563			

Question 6:-

a) $$f_a \propto \int_r^R dr\, r^2 \rho(r) \int_0^{\pi} d\phi \sin\phi\, e^{-i\frac{4\pi}{\lambda}\sin\theta\cos\phi}$$

$$\mu \equiv \frac{4\pi}{\lambda}\sin\theta$$

$$A = \int_0^{\pi} d\phi \sin\phi\, e^{-i\mu\cos\phi}$$

$$u = -\cos\phi \quad ; \quad du = \sin\phi\, d\phi$$

$$A = \int_{-1}^{1} du\, e^{i\mu u} = \frac{1}{i\mu} e^{i\mu u}\Big|_{-1}^{1} = \frac{2}{\mu}\frac{(e^{i\mu} - e^{-i\mu})}{2i}$$

$$= 2\frac{\sin(\mu)}{\mu} = 2\,\mathrm{sinc}(\mu)$$ ✓

b) $$\rho(r) = \beta e^{-r/b}$$

$$f_a = \gamma \int_r^R dr\, r^2 \beta e^{-r/b}\, 2\,\mathrm{sinc}(\mu)$$ ✓

$$= 2\gamma\beta\,\mathrm{sinc}(\mu) \int_r^R dr\, r^2 e^{-r/b}$$ ✓

$$\Rightarrow \int_r^R dr\, r^2 e^{-r/b} = \int_r^R dr\, r^2 \frac{d}{dr}\left(-b e^{-r/b}\right)$$

$$= \left[-b r^2 e^{-r/b}\right]_r^R + 2b\int_r^R dr\, r e^{-r/b}$$

$$= \left[-b r^2 e^{-r/b}\right]_r^R + 2b\int_r^R dr\, r \frac{d}{dr}\left(-b e^{-r/b}\right)$$

$$= -b\left[r^2 e^{-r/b}\right]_r^R - 2b^2\left[r e^{-r/b}\right]_r^R +$$

$$+ 2b^2 \int_r^R dr\, e^{-r/b}$$

$$= -b\left\{ 2b^2 e^{-R/b} - 2b^2 e^{-r/b} + R^2 e^{-R/b} - r^2 e^{-r/b} + \right.$$
$$\left. + 2b R e^{-R/b} - 2br e^{-r/b} \right\}$$

$$= b\left\{ \left(r^2 + 2br + 2b^2\right) e^{-r/b} + \right.$$
$$\left. - \left(R^2 + 2bR + 2b^2\right) e^{-R/b} \right\}$$

$$f_a = 2\gamma\beta b \,\mathrm{sinc}(\mu) \underbrace{\left\{ \left(r^2 + 2br + 2b^2\right) e^{-r/b} + - \left(R^2 + 2bR + 2b^2\right) e^{-R/b} \right\}}$$

$$\frac{2 + e^{-bR}\left(-2 - bR\,(2 + bR)\right)}{b^3}$$

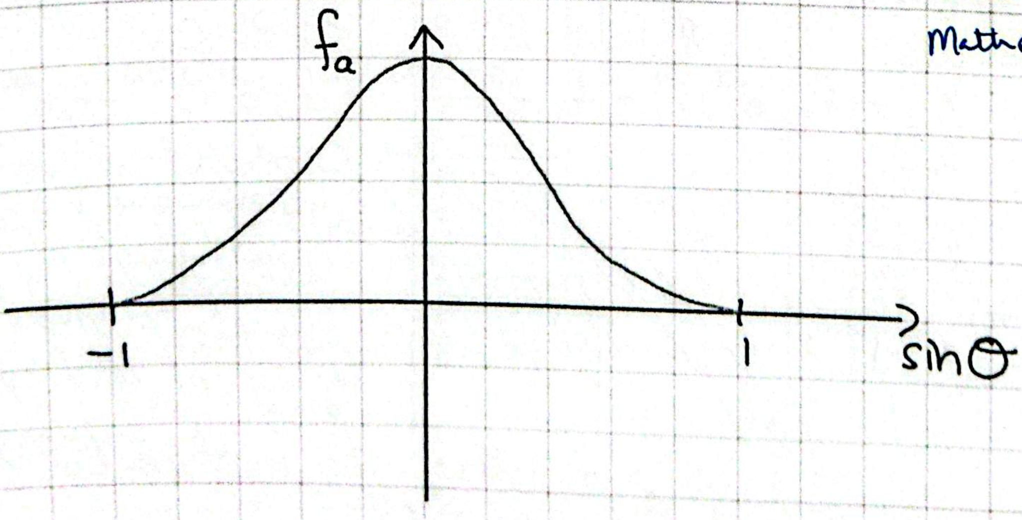
Computed with Mathematica.

c) $f_a \propto \mathrm{sinc}(\mu) = \dfrac{\sin(\mu)}{\mu}$ ✓

where $\mu = \dfrac{4\pi}{\lambda} \sin\theta$

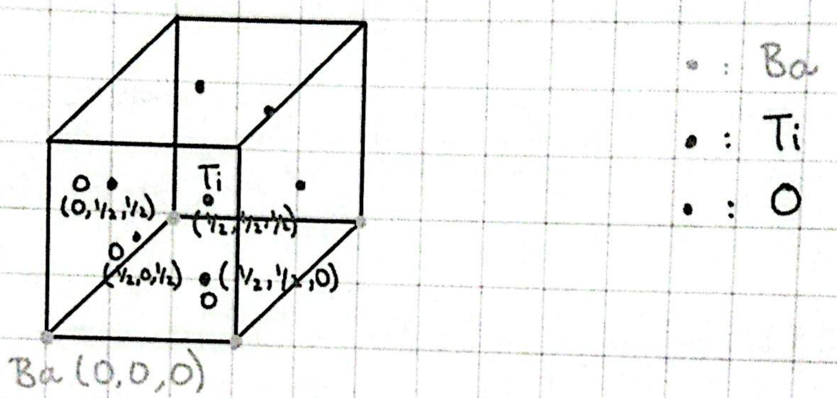
$$f_a \propto \frac{\lambda}{4\pi \sin\theta} \sin\left[\frac{4\pi}{\lambda} \sin\theta\right]$$ ✓

$$\propto \frac{1}{\sin\theta} \sin\left[\frac{4\pi}{\lambda} \sin\theta\right]$$



Question 7:-

a)



b)

$$S_{hkl} = S_{lattice}\, S_{basis}$$

$S_{lattice} = 1$ for a primitive cubic structure

$$\Rightarrow S_{hkl} = S_{basis}$$
$$= \sum_j f_j \exp\left[2\pi i\left(hx_j + ky_j + lz_j\right)\right]$$

$$S_{(00l)} = \sum_j f_j\, e^{2\pi i l z_j}$$

$$= f_{Ba}\, e^{2\pi i(0)} + f_{Ti}\, e^{2\pi i(l/2)} + f_O\, e^{2\pi i(l/2)} + f_O\, e^{2\pi i(l/2)}$$

~~seemingly BCC structure where~~ $\cancel{\lim_{\substack{h\to 0\\ k\to 0}} f_{Ti}\, e^{2\pi i(h+k+l)/2}}$

~~seemingly FCC structure where~~ $\cancel{\lim_{\substack{h\to 0\\ k\to 0}} f_O e^{2\pi i(h+k)/2} + f_O e^{2\pi i(h+l)/2} + f_O e^{2\pi i(k+l)/2}}$

with $l = 1$

$$e^{2\pi i(l/2)} = e^{\pi i} = -1$$

with $l = 1$

$$e^{2\pi i(l/2)} = -1$$

$$= f_{Ba} + (-1)^l f_{Ti} + 2(-1)^l f_O$$

$$\therefore \boxed{S_{(001)} = f_{Ba} - f_{Ti} - 2f_O}$$

tion 8:-

Bragg's Law:-

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

For $n=1$: $2d\sin\theta = \lambda$

For a cubic structure: $d^2 = \frac{a^2}{\sqrt{h^2+k^2+l^2}} = \frac{a^2}{\sqrt{N}}$,

where $N = h^2+k^2+l^2$.

$$\Rightarrow 2\frac{a^2}{\sqrt{N}}\sin\theta = \lambda$$

$$\therefore \sin^2\theta = \frac{\lambda^2}{4a^2}N = AN \quad \left(\text{where } A = \frac{\lambda^2}{4a^2}\right)$$

b)

$\sin^2\theta$	N	$\times 3$	hkl
0.1365	$\frac{0.1365}{0.1365} = 1$	3	(111)
0.1820	$\frac{0.1820}{0.1365} = \frac{4}{3}$	4	(200)
0.3640	$\frac{0.3640}{0.1365} = \frac{8}{3}$	8	(220)
0.5005	$\frac{0.5005}{0.1365} = \frac{11}{3}$	11	(311)
0.5460	$\frac{0.5460}{0.1365} = 4$	12	(222)
0.7280	$\frac{0.7280}{0.1365} = \frac{16}{3}$	16	(400)
0.8645	$\frac{0.8645}{0.1365} = \frac{19}{3}$	19	(331)
0.9100	$\frac{0.9100}{0.1365} = \frac{20}{3}$	20	(420)

✓ Note that even and odd do not mix, as this is face-centred.

To find the unit cell: $a = \frac{\lambda}{2}\frac{1}{\sqrt{A}}$

where $A = \frac{0.1365}{3} = \frac{0.1820}{4} = \frac{0.3640}{8} = \ldots$

$= 0.0455$

$\therefore \quad a = \frac{\lambda}{2\sqrt{A}} = \frac{154}{2\sqrt{0.0455}}$ pm stion 9:-

C atom at (0,0,0)

After FCC translation → Possible positions: (0,0,0), (0,1/2,1/2), (1/2,0,1/2), (1/2,1/2,0).

C atom at (1/4,1/4,1/4)

After FCC translation → Possible positions: (1/4,1/4,1/4), (1/4,3/4,3/4), (3/4,1/4,3/4), (3/4,3/4,1/4)

∴ There are 8 equivalent positions:-

(0,0,0), (0,1/2,1/2), (1/2,0,1/2), (1/2,1/2,0),
(1/4,1/4,1/4), (1/4,3/4,3/4), (3/4,1/4,3/4), (3/4,3/4,1/4) $\boxed{\text{Set A}}$

8a Wycoff positions are {(0,0,0), (3/4,1/4,3/4)}

$\{+(0,0,0), +(0,\frac{1}{2},\frac{1}{2}), +(\frac{1}{2},0,\frac{1}{2}), +(\frac{1}{2},\frac{1}{2},0)\}$ we can add these translations and find the positions which would turn out to be identical to set $\boxed{A}$. I require you to show the complete working.

XX Since (3/4,1/4,3/4) and ~~(1/4,1/4,1/4) are equivalent positions, these positions can be generated with basis set of (0,0,0) & (1/4,1/4,1/4)~~

b) $$S_{hkl}^{basis} = f_c \sum_j e^{2\pi i(hx_j+ky_j+lz_j)}$$

$$= f_c\left[e^{2\pi i(0,0,0)} + e^{2\pi i(h+k+l)/4}\right]$$

$$= f_c\left[1 + e^{\pi i(h+k+l)/2}\right]$$

$$= \begin{cases} 2f_c & h+k+l = 2n \text{ where } n \text{ is even} \\ f_c(1+i) & h+k+l = 1 \pmod 4 \\ 0 & h+k+l = 2n \text{ where } n \text{ is odd} \\ f_c(1-i) & h+k+l = 3 \pmod 4 \end{cases}$$

$\therefore$ S_{hkl} systematic absence at $h+k+l = 2n$ (where n is odd) by the S_{hkl}^{basis}

Similarly $S_{hkl}^{lattice} = 1 + e^{i\pi(h+k)} + e^{i\pi(k+l)} + e^{i\pi(h+l)}$

↳ as it is an FCC structure

$$= \begin{cases} \text{non-zero} & h+k+l = 2n \\ \text{non-zero} & h+k+l = 2n+1 \\ 0 & \text{otherwise} \end{cases}$$

(meaning if all h, k, l indices are mixed odd/even)

$\therefore$ Systematic absences occur:

$$= \begin{cases} h,k,l \text{ are mixed odd/even indices} & \text{(due to lattice)} \\ h+k+l = 2n \text{ where } n \text{ is odd} & \text{(due to basis)} \end{cases}$$

c) $I \propto |S_{hkl}^{basis}|^2 = 4f_c^2$ $\quad h+k+l = 2n$ where n is even

$I \propto |S_{hkl}^{basis}|^2 = f_c^2|1+i|^2$ $\quad h+k+l = 1 \pmod 4$

$= f_c^2(1+i)(1-i)$

$$= 2f_c^2$$

$$I \propto |S_{hkl}^{basis}|^2 = f_c^2 |1-i|^2 \qquad h+k+l = 3 \pmod 4$$
$$= f_c^2 (1-i)(1+i)$$
$$= 2f_c^2$$

$$\Rightarrow \quad I \propto \begin{cases} 4f_c^2 & h+k+l = 2n \text{ where } n \text{ is even} \\ 2f_c^2 & h+k+l = 2n+1 \end{cases}$$