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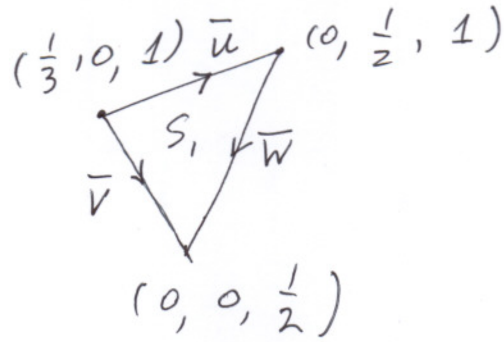
# FSK 324 Test 1 - Memorandum
## (Solid State Physics)

* Please note:

> There are several solutions. ONLY two methods are shown here.

## A. Crystal structure

**Q1.** For plane $S_1$




It is therefore possible to find three vectors, $\bar{u}$, $\bar{v}$ and $\bar{w}$ on $S_1$. Any two pairs generate the perpendicular direction, from which the Miller indices can be (deduced) computed. For instance:

$$\bar{u} = \left(0 - \tfrac{1}{3},\ \tfrac{1}{2} - 0,\ 1 - 1\right) = \left(-\tfrac{1}{3},\ \tfrac{1}{2},\ 0\right)$$

$$\bar{v} = \left(0 - \tfrac{1}{3},\ 0 - 0,\ \tfrac{1}{2} - 1\right) = \left(-\tfrac{1}{3},\ 0,\ -\tfrac{1}{2}\right)$$

$$\bar{w} = \left(0 - 0,\ 0 - \tfrac{1}{2},\ \tfrac{1}{2} - 1\right) = \left(0,\ -\tfrac{1}{2},\ -\tfrac{1}{2}\right)$$

Taking $\bar{u}$ and $\bar{v}$:

$$\Rightarrow \text{Let } \bar{p} = \bar{v} \wedge \bar{u} = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ -\frac{1}{3} & 0 & -\frac{1}{2} \\ -\frac{1}{3} & \frac{1}{2} & 0 \end{vmatrix}$$

$$= \hat{i}\left(0 - \left(\tfrac{1}{2}\right)\left(-\tfrac{1}{2}\right)\right) - \hat{j}\left(0 - \left(-\tfrac{1}{3}\right)\left(-\tfrac{1}{2}\right)\right) + \hat{k}\left(\left(-\tfrac{1}{3}\right)\left(\tfrac{1}{2}\right) - 0\right)$$

$$= \frac{1}{4}\hat{i} + \frac{1}{6}\hat{j} - \frac{1}{6}\hat{k}$$

Hence a vector perpendicular to $S_1$ is

$$\bar{p} = \left(\frac{1}{4}, \frac{1}{6}, -\frac{1}{6}\right)$$

Since <u>ONLY</u> direction is being considered, scaling $\bar{p}$ to a new vector $\bar{p}' = LCM(4,6,6) * \bar{p}$ produces another parallel vector.

$$\Rightarrow \quad \bar{p}' = 12\left(\frac{1}{4}, \frac{1}{6}, -\frac{1}{6}\right)$$

$$= (3, 2, -2)$$ , measured from the origin.

Hence the plane $S_1$ can also be described by $(3\,2\,\bar{2})$

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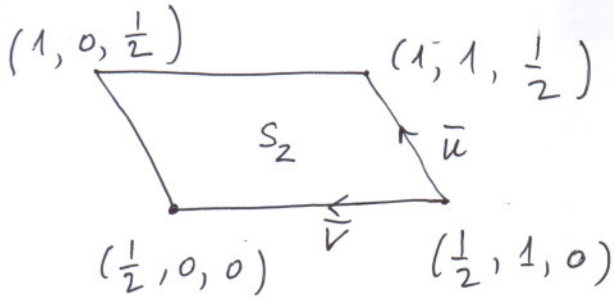
An alternate method (which <u>you FSK324</u> students can try) is:

| | $x$: | $y$: | $z$: |
|---|---|---|---|
| Intercepts of $S_1$: | $\frac{a}{3}$ | $\frac{b}{2}$ | $-\frac{c}{2}$ |
| $\Downarrow$ | $\frac{1}{3}$ | $\frac{1}{2}$ | $-\frac{1}{2}$ |
| $\overline{\Downarrow}$ | $\frac{3}{1}$ | $\frac{2}{1}$ | $-\frac{2}{1}$ |
| $\overline{\Downarrow}$ | $(3$ | $2$ | $\bar{2})$. |

(<u>Easy, right?</u>)

For plane $S_2$




Long (general) method:

$$\bar{u} = (1, 1, \tfrac{1}{2}) - (\tfrac{1}{2}, 1, 0)$$

$$= (\tfrac{1}{2}, 0, \tfrac{1}{2})$$

$$\bar{v} = (\tfrac{1}{2}, 0, 0) - (\tfrac{1}{2}, 1, 0)$$

$$= (0, -1, 0)$$

$$\therefore \bar{p} = \bar{u} \wedge \bar{v} = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ \frac{1}{2} & 0 & \frac{1}{2} \\ 0 & -1 & 0 \end{vmatrix}$$

$$= \hat{i}\left[0 - (-1)(\tfrac{1}{2})\right] - \hat{j}\left[0 - 0\right] + \hat{k}\left[(\cancel{-1})(\tfrac{1}{2}) - 0\right]$$

$$= \frac{1}{2}\hat{i} + 0\hat{j} + \left(-\frac{\cancel{1}}{2}\right)\hat{k}$$

$$= \left(\frac{1}{2}, 0, -\frac{\cancel{1}}{2}\right)$$

Hence scaling by the LCM (i.e. a factor of 2) gives

$$\bar{p}' = (1, 0, -\cancel{1})$$

which is perpendicular to

$S_2 = (1\ 0\ \bar{1})$ and also to

$(\bar{1}\ 0\ 1)$.

## Method 2

| | $x$: | $y$: | $z$: |
|---|---|---|---|
| Intercepts: | $-\frac{a}{2}$ | $\infty . b$ | $\frac{c}{2}$ |
| $\Downarrow$ | $-\frac{1}{2}$ | $\frac{\infty}{1}$ | $\frac{1}{2}$ |
| $\Downarrow$ | $-\frac{2}{1}$ | $\frac{1}{\infty}$ | $\frac{2}{1}$ |
| $\Downarrow$ | $-2$ | $0$ | $2$ |
| (Reduce) | $-1$ | $0$ | $1$ |

$$\Downarrow$$

$$(\bar{1}\ 0\ 1).$$

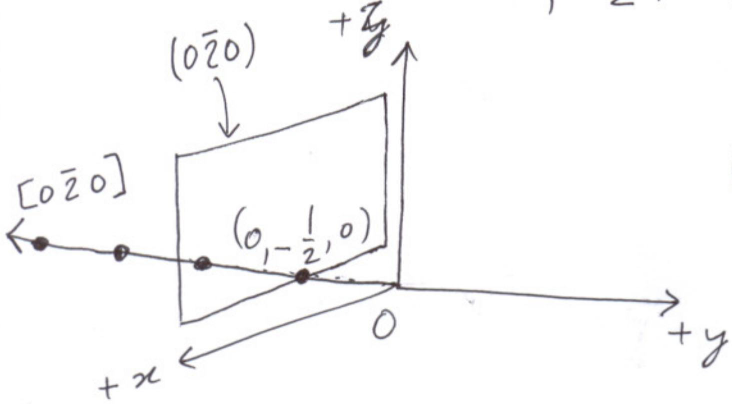
Note:

Method 1 is general enough to find all planes equivalent to S2. Method 2 finds only one plane. Some extrapolation is needed to find others.

Q2. $(0\ \bar{2}\ 0)$ is a plane

(i) $\therefore (0\ \bar{2}\ 0) \to (0\ \ -2\ \ 0) \to \left(\frac{0}{1}\ \ \frac{-2}{1}\ \ \frac{0}{1}\right)$

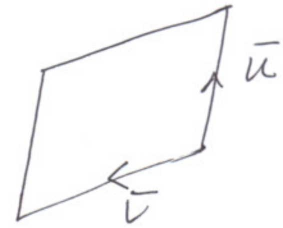
$$(\infty, -\tfrac{1}{2}, \infty) \leftarrow \left(\frac{1}{0}, -\frac{1}{2}, \frac{1}{0}\right)$$




(ii) $[0\ \bar{2}\ 0]$ is a directed line segment from $0$ to $(0, -2, 0)$.

(iii) Consider any two arbitrary vectors $\bar{u}$ and $\bar{v}$ on the $(0\,\bar{2}\,0)$ plane. For instance, let

$\bar{u} = (b_1\hat{i} + b_2\hat{j} + 0\hat{k})$ and $\bar{v} = (a_1\hat{i} + a_2\hat{j} + 0\hat{k})$.




where $a_1, a_2, b_1, b_2 \neq 0$.

Let $\bar{w} = \bar{u} \wedge \bar{v}$,

$$\Rightarrow \bar{w} = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ b_1 & b_2 & 0 \\ a_1 & a_2 & 0 \end{vmatrix}$$

$$= 0\hat{i} + 0\hat{j} + (a_2 b_1 - a_1 b_2)\hat{k}$$

Let $\bar{p} = [0\,\bar{2}\,0] = -2\hat{j}$

<u>Hypothesis:</u>

If $\bar{p} \cdot \bar{w} = 0$, then $\bar{p} \perp \bar{w}$, $\forall a_1, a_2, b_1, b_2 \neq 0$.

<u>Check hypothesis:</u>

$$\bar{p} \cdot \bar{w} = (0, -2, 0) \cdot (0, 0, (a_2 b_1 - a_1 b_2))$$

$$= 0$$

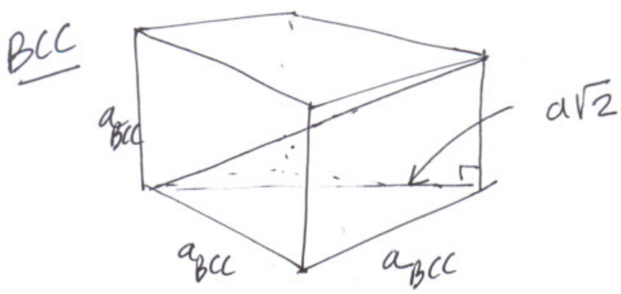
$$= |\bar{p}||\bar{w}| \cos\phi = pw\cos\phi$$

$\therefore \cos\phi = 0$ since $p, w \neq 0$.

$\Rightarrow \underline{\underline{\phi = 90^\circ}}$, hence the plane $(0\,\bar{2}\,0)$ is perpendicular to the $[0\,\bar{2}\,0]$ direction.

Q3. Method : use the BCC structure to determine the atomic radius of iron, then use it in the FCC structure.

BCC




Body-diagonal length :

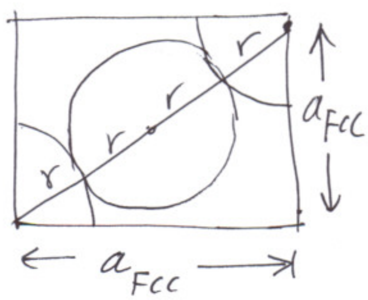
$$= \sqrt{a_{BCC}^2 + 2a_{BCC}^2}$$

$$= a_{BCC}\sqrt{3}$$

$$= 4r$$

$$\therefore\ r = \frac{a\sqrt{3}}{4} \quad \left(= \frac{0.286\sqrt{3}}{4}\,nm = 0.1238\,nm\right)$$

Side of FCC




Face diagonal length

$$= 4r$$

$$= a_{BCC}\sqrt{3}$$

$$= \sqrt{a_{FCC}^2 + a_{FCC}^2}$$

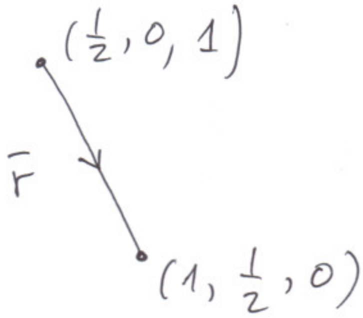
$$= a_{FCC}\sqrt{2}$$

$$\Rightarrow a_{FCC} = a_{BCC}\sqrt{\frac{3}{2}} = 0.286\sqrt{\frac{3}{2}}\ (nm)$$

$$= 0.3503\,nm$$

$$\approx \underline{\underline{0.35\,nm}}$$

**Q4.**




$$\Rightarrow \bar{r} = \left(1, \tfrac{1}{2}, 0\right) - \left(\tfrac{1}{2}, 0, 1\right)$$

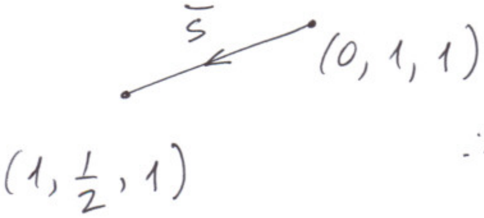
$$= \left(1 - \tfrac{1}{2},\ \tfrac{1}{2} - 0,\ 0 - 1\right)$$

$$= \left(\tfrac{1}{2},\ \tfrac{1}{2},\ -1\right)$$

Hence the index is $(LCM * \bar{r})$

$$\therefore \bar{r} = (1, 1, -2)$$

$$= [1\ 1\ \bar{2}].$$

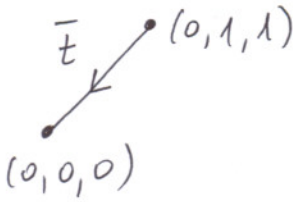



$$\therefore \bar{s} = \left(1 - 0,\ \tfrac{1}{2} - 1,\ 1 - 1\right)$$

$$= \left(1, -\tfrac{1}{2}, 0\right)$$

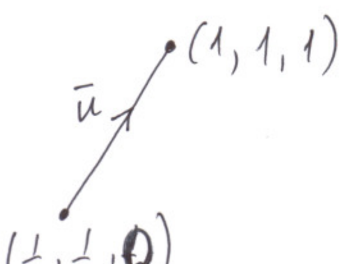
$$\equiv (2, -1, 0)$$

Hence $\bar{s} = [2\ \bar{1}\ 0]$.




$$\therefore \bar{t} = (0-0,\ 0-1,\ 0-1) = (0, -1, -1)$$

$$\equiv [0\ \bar{1}\ \bar{1}].$$




$$\Rightarrow \bar{u} = \left(1 - \tfrac{1}{2},\ 1 - \tfrac{1}{2},\ 1 - 0\right) = \left(\tfrac{1}{2}, \tfrac{1}{2}, 1\right)$$

$$\equiv [1\ 1\ 2].$$

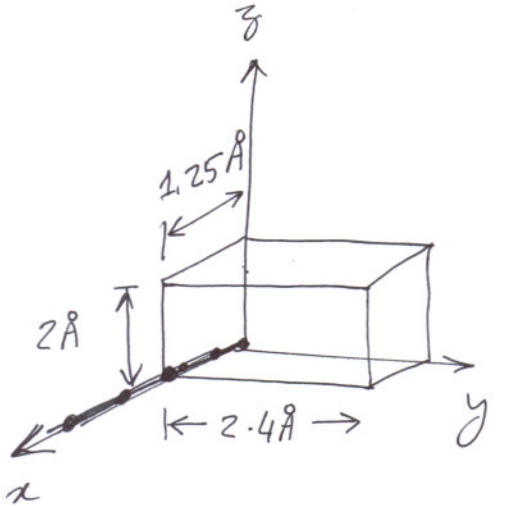
Q5.

$$\bar{a}_1 = a\hat{i} = 1.25\hat{i} = (1.25, 0, 0)$$

$$\bar{a}_2 = b\hat{j} = 2.4\hat{j} = (0, 2.4, 0)$$

$$\bar{a}_3 = c\hat{k} = 2.0\hat{k} = (0, 0, 2).$$

$$V_c = \bar{a}_1 \cdot (\bar{a}_2 \wedge \bar{a}_3) = (1.25, 0, 0) \cdot \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ 0 & 2.4 & 0 \\ 0 & 0 & 2 \end{vmatrix}$$




$$= (1.25, 0, 0) \cdot (4.8, 0, 0)$$

$$= 1.25(4.8)\,Å^3$$

$$= \underline{\underline{6\,Å^3}}.$$

Reciprocal lattice:

$$\bar{b}_1 = \frac{2\pi}{V_c}(\bar{a}_2 \wedge \bar{a}_3)\,;\ \bar{b}_2 = \frac{2\pi}{V_c}(\bar{a}_3 \wedge \bar{a}_1)\,;\ \bar{b}_3 = \frac{2\pi}{V_c}(\bar{a}_1 \wedge \bar{a}_2)$$

$$\bar{a}_2 \wedge \bar{a}_3 = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ 0 & 2.4 & 0 \\ 0 & 0 & 2 \end{vmatrix} = (4.8, 0, 0)$$

$$\Rightarrow \bar{b}_1 = \frac{2\pi}{6}(4.8, 0, 0) = (1.6\pi, 0, 0)$$

$$\bar{a}_3 \wedge \bar{a}_1 = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ 0 & 0 & 2 \\ 1.25 & 0 & 0 \end{vmatrix} = (0, 2.5, 0)$$

$$\therefore \bar{b}_2 = \frac{2\pi}{6}(0, 2.5, 0) = (0, \frac{5\pi}{6}, 0)$$

$$\bar{a}_1 \wedge \bar{a}_2 = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ 1.25 & 0 & 0 \\ 0 & 2.4 & 0 \end{vmatrix} = (0, 0, 3) \Rightarrow \bar{b}_3 = \frac{2\pi}{6}(0, 0, 3) = (0, 0, \pi).$$

$$V_c' = \bar{b}_1 \cdot (\bar{b}_2 \wedge \bar{b}_3)$$

$$= (1.6\pi, 0, 0) \cdot \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ 0 & \frac{5\pi}{6} & 0 \\ 0 & 0 & \pi \end{vmatrix}$$

$$= (1.6\pi, 0, 0) \cdot \left(\frac{5\pi^2}{6}, 0, 0\right)$$

$$= \frac{8}{6}\pi^3 \text{Å}^3$$

Hence $\frac{V_c}{V_c^{*\prime}} = \frac{6}{\frac{8\pi^3}{6}} = \frac{9}{2\pi^3}$.

Q6. $E = 8056\,eV = h\frac{c}{\lambda}$

$1\,eV = 1.6022 \times 10^{-19}\,J$

$\therefore 8056\,eV = 1.2907 \times 10^{-15}\,J = h\frac{c}{\lambda}$

$\Rightarrow \lambda = \frac{6.626 \times 10^{-34} \times 3 \times 10^{8}}{1.2907 \times 10^{-15}}\,m = 1.54 \times 10^{-10}\,m$

(1.54 Å).

Bragg's law $\Rightarrow$ $n\lambda = 2d\sin\theta$

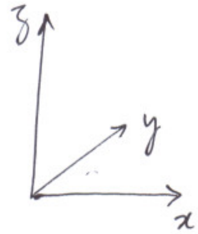
$$d = \frac{a}{\sqrt{h^2+k^2+l^2}}$$

$$= \frac{2.42\ (\text{Å})}{\sqrt{h^2+k^2+l^2}}$$

| (hkl) | d (Å) | $n=1$, $\sin\theta = \frac{\lambda}{2d}$ |
|---|---|---|
| (100) | 2.42 | $\theta = 18.55°$ |
| (200) | 1.21 | $\theta = 39.52°$ |
| (211) | 0.988 | $\theta = 51.20°$ |

Q7. For the FCC, the indicated atoms have the fractional coordinates:

$$(0,0,0),\ \left(\tfrac{1}{2},\tfrac{1}{2},0\right),\ \left(\tfrac{1}{2},0,\tfrac{1}{2}\right),\ \left(0,\tfrac{1}{2},\tfrac{1}{2}\right)$$




Given reflections of the form $(v_1\, v_2\, v_3)$, then

$$S_{\bar{G}(v_1 v_2 v_3)} = \sum_{j=1}^{N} f_j\, e^{-i2\pi(v_1 x_j + v_2 y_j + v_3 z_j)}$$

Hence for the indicated FCC atoms, $N=4$

$$\Rightarrow S_{\bar{G}(v_1 v_2 v_3)} = \sum_{j=1}^{4} f_j \left[ e^{-2\pi i(v_1 x_j + v_2 y_j + v_3 z_j)} \right]$$

$$\boxed{\text{If } f = f_j,\ \forall j \in \{1,2,3,4\},\ \text{then}}$$

$$S_{\bar{G}(v_1 v_2 v_3)} = \underset{\substack{\uparrow \\ j=1}}{f e^{-2\pi i(0)}} + \underset{\substack{\uparrow \\ j=2}}{f e^{-2\pi i\left(\frac{v_1}{2}+\frac{v_2}{2}\right)}} + \underset{\substack{\uparrow \\ j=3}}{f e^{-2\pi i\left(\frac{v_1}{2}+\frac{v_3}{2}\right)}}$$

$$+ f e^{-2\pi i\left(\frac{v_2}{2}+\frac{v_3}{2}\right)}$$

$$= \underset{\substack{\uparrow \\ \text{term 1}}}{f} + \underbrace{f e^{-\pi i(v_1+v_2)}}_{\text{term 2}} + \underbrace{f e^{-\pi i(v_1+v_3)}}_{\text{term 3}} + \underbrace{f e^{-\pi i(v_2+v_3)}}_{\text{term 4}}$$

Note: Since $V_1, V_2, V_3$ are all integers, any sum of $V_1, V_2, V_3$ is also integer. That is, ~~for~~ for FCC, let

$$a=(V_1+V_2),\quad b=(V_1+V_3) \text{ and } c=(V_2+V_3),$$

where $a, b, c \in \mathbb{Z}$.

Then

$$S_{\bar{G}}(V_1V_2V_3) = \underset{\substack{T1\\(\text{term }1)}}{f} + \underset{\substack{T2\\(\text{term }2)}}{f(-1)^a} + \underset{\substack{T_3\\(\text{term }3)}}{f(-1)^b} + \underset{\substack{T_4\\(\text{term }4)}}{f(-1)^c}.$$

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* For any of you STUDENTS who STILL don't get the LOGIC, let's build up a "logic" table as follows:

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Let "0" ⇒ index / sum is even; "1" ⇒ index/sum is odd.

For the FCC structure factor above, there are 8-possibilities

| ← indices → | | | ← sums → | | | ← Terms of $S_{\bar{G}}$ → | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| $V_1$ | $V_2$ | $V_3$ | $V_1+V_2$ | $V_1+V_3$ | $V_2+V_3$ | $T_1$ | $T_2$ | $T_3$ | $T_4$ | $S_{\bar{G}}$ |
| 0 | 0 | 0 | 0 | 0 | 0 | f | f | f | f | 4f |
| 0 | 0 | 1 | 0 | 1 | 1 | f | f | −f | −f | 0 |
| 0 | 1 | 0 | 1 | 0 | 1 | f | −f | f | −f | 0 |
| 0 | 1 | 1 | 1 | 1 | 0 | f | −f | −f | f | 0 |
| 1 | 0 | 0 | 1 | 1 | 0 | f | −f | −f | f | 0 |
| 1 | 0 | 1 | 1 | 0 | 1 | f | −f | +f | −f | 0 |
| 1 | 1 | 0 | 0 | 1 | 1 | f | f | −f | −f | 0 |
| 1 | 1 | 1 | 0 | 0 | 0 | f | f | f | f | 4f |

all "even"

all "ODD"

$S_{\bar{G}} = T_1+T_2+T_3+T_4$

Hence $S_{\bar{G}} = 0$ if NOT all even or odd.

For BCC, the fractional coordinates are:

$$\underbrace{(0,0,0)}_{1^{st}} \text{ and } \underbrace{\left(\frac{1}{2},\frac{1}{2},\frac{1}{2}\right)}_{2^{nd}} \Rightarrow N=2$$

$$\therefore \quad S_{\bar{G}}(v_1 v_2 v_3) = \sum_{j=1}^{2} f_j \, e^{-2\pi i (v_1 x_j + v_2 y_j + v_3 z_j)}$$

Then if $f_j = f, \forall j$ then

$$S_{\bar{G}}(v_1 v_2 v_3) = \underset{\uparrow T_1}{f} e^{-2\pi i(0+0+0)} + \underset{\uparrow T_2}{f} e^{-2\pi i\left(\frac{v_1+v_2+v_3}{2}\right)}$$

$$= f e^{0} + f e^{-\pi i (v_1+v_2+v_3)}$$

$$= f + f\left(e^{-\pi i}\right)^{a}$$

$$= f + f(-1)^{a} \quad \text{where } a = (v_1+v_2+v_3)$$

If $a$ is even, then $S_{\bar{G}}(v_1 v_2 v_3) = f + f = 2f$

If $a$ is odd, then $S_{\bar{G}}(v_1 v_2 v_3) = f - f = 0$.

These conditions hold when:

ALL $v_1, v_2, v_3$ are even or ~~all~~ two odd then $a$ is even

$\Rightarrow S_{\bar{G}}(v_1 v_2 v_3) = 2f$.

Otherwise (i.e. if there is at least one odd and some even, OR at least one even and some odd)

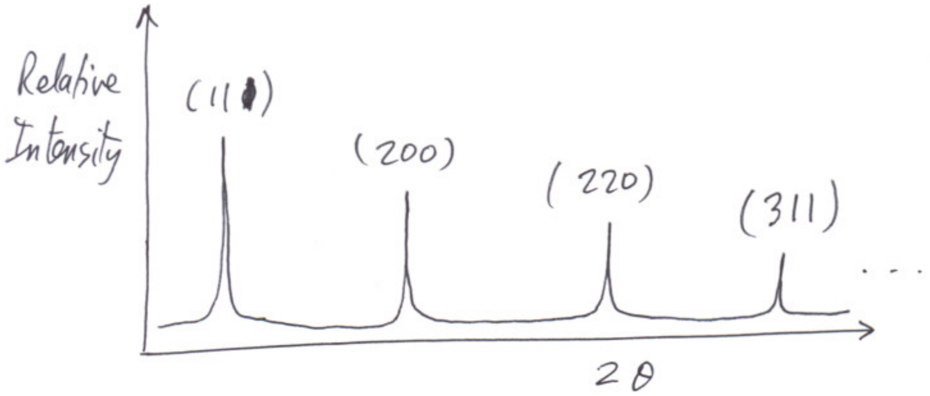
then $S_{\bar{G}}(v_1 v_2 v_3) = 0$.

For instance: (111), (200), (

**Q8.** $n\lambda = 2d\sin\theta$

Note that for the FCC structure, the only allowable reflections occur when $(h, k, l)$ are either all <u>odd</u> or all even. That is:

$$(1\,1\,1),\ (2\,0\,0),\ (2\,2\,0),$$
$$(3\,1\,1),\ (3\,3\,1),\ \ldots$$




FCC

(see also Table 1, Question 7).

(i) Hence we see that the following table results:

| ≈ 2θ | ≈ θ | h k l | $d = \frac{n\lambda}{2\sin\theta}$, n = 1 |
|---|---|---|---|
| 43° | 21.5° | 1 1 1 | $\frac{1 \times 0.1542}{2\sin 21.5°} \approx 0.2081$ nm |
| 51° | 25.5° | 2 0 0 | 0.179 nm |
| 74° | 37.0° | 2 2 0 | 0.1281 nm |
| 91° | 45.5° | 3 1 1 | 0.1081 nm |
| ⋮ | ⋮ | 3 3 1 | ⋮ |

Try listing them to see for yourself:

| | | Reason |
|---|---|---|
| (1 0 0) | × | odd even even |
| (1 0 1) | × | odd even odd |
| (1 1 0) | × | odd odd even |
| (1 1 1) | ✓ | odd odd odd |
| (2 0 0) | ✓ | even even even |
| (2 0 1) | × | even even odd |
| (2 1 0) | × | even odd even |
| (2 1 1) | × | even odd odd |
| (2 2 0) | ✓ | even even even |
| (2 2 1) | × | even even odd |
| (2 2 2) | ✓ | even even even |
| (3 0 0) | × | odd even even |
| (3 1 1) | ✓ | odd odd odd |
| ⋮ | | |
| (3 3 [redacted]) | ✓ | odd odd odd |
| ⋮ | | |

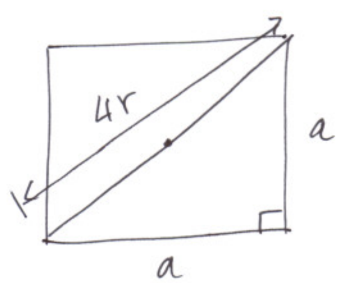
and so on.

(ii) But $d = \dfrac{a}{\sqrt{h^2+k^2+l^2}} \Rightarrow a = d\sqrt{h^2+k^2+l^2}$

$\therefore$

| (h k l) | d (nm) | a (nm) | r (nm) |
|---|---|---|---|
| (1 1 1) | 0.2081 | $a = 0.2081\sqrt{1^2+1^2+1^2} = 0.3604$ | 0.1274 |
| (2 0 0) | 0.1791 | $a = 0.1791\sqrt{2^2+0^2+0^2} = 0.3582$ | 0.1266 |
| (2 2 0) | 0.1281 | $a = 0.1281\sqrt{2^2+2^2+0^2} = 0.3624$ | 0.1281 |
| 3 1 1 | 0.1081 | $a = 0.1081\sqrt{3^2+1^2+1^2} = 0.3582$ | 0.1268 |

(iii) for FCC, taking one-face diagonal




$$(4r)^2 = a^2 + a^2$$

$$\Rightarrow 16r^2 = 2a^2$$

$$\therefore r = \frac{a}{\sqrt{8}}$$

For example, for $(hkl) = (111)$,

$$r = \frac{0.3604}{\sqrt{8}}\,nm = 0.1274\,nm$$

<u>Note:</u> From the literature, the atomic radius of copper is <u>0.128 nm</u>.

——— end of test ———