Section A:

1. (i) Amorphous materials — are materials with no long range ordering, although there may be short range ordering.

Example: glass

(ii) Schottky defect — is a type of defect in a lattice in which an atom leaves its equilibrium position and sits on the surface.

Application: Semiconductor devices.

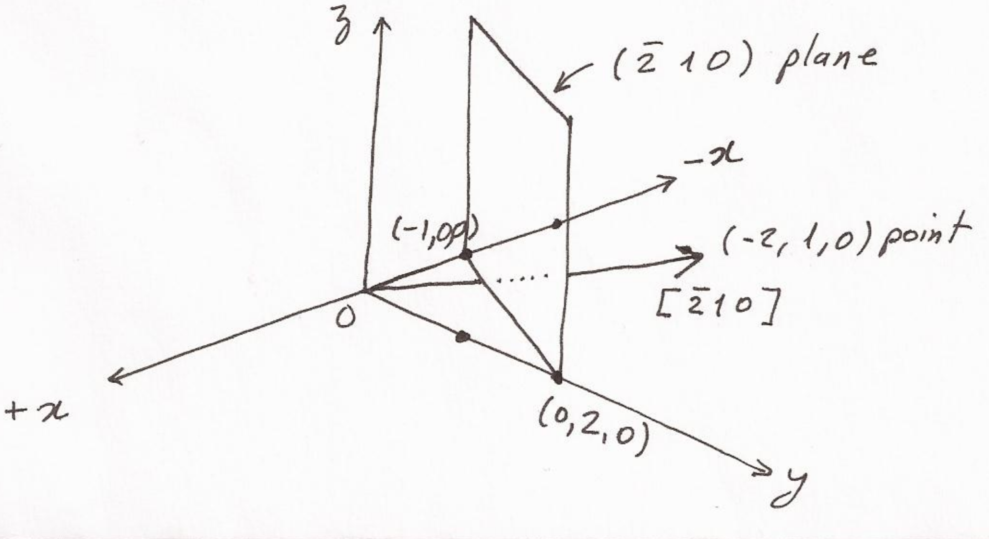
2. (i) $(\bar{2}\ 1\ 0) = (-2\ 1\ 0)$ represents a plane.

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

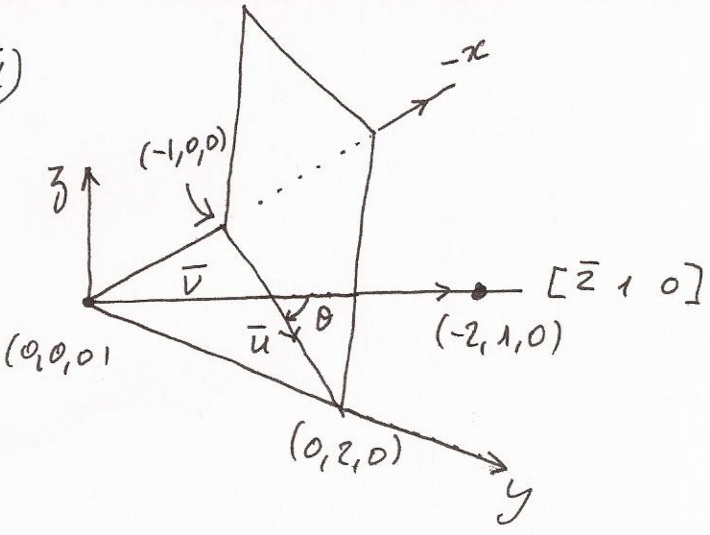
$$\downarrow$$

$$\begin{matrix}(-1 & 2 & \infty) \\ (x & y & z)\end{matrix} \leftarrow \left(-\tfrac{1}{2}\ 1\ \infty\right)$$

(ii) $[\bar{2}\ 1\ 0] \Rightarrow$ a direction i.e. the line joining $(0,0,0)$ and $(-2,1,0)$ points.



(iii)



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

$= (1, 2, 0)$

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

i.e. $= (-2,1,0) - (0,0,0)$

$= (-2, 1, 0)$

Then $\bar{u} \cdot \bar{v} = |\bar{u}||\bar{v}| \cos\theta$

$$[1(-2) + 2(1) + 0(0)] = \sqrt{1^2+2^2+0^2}\sqrt{(-2)^2+1^2+0^2}\ \cos\theta$$

$$\therefore \quad 0 = 5\cos\theta$$

$$\Rightarrow \cos\theta = 0$$

$$\Rightarrow \theta = \cos^{-1}(0)$$

$$= 90^\circ$$

Hence vectors $\bar{u}$ and $\bar{v}$ are perpendicular

$\Rightarrow$ $[\bar{2}\ 1\ 0]$ and $(\bar{2}\ 1\ 0)$ are perpendicular.

<u>Note</u>:
Vector $\bar{u}$ lies on the plane $(\bar{2}\ 1\ 0)$ and vector $\bar{v}$ is in the direction $[\bar{2}\ 1\ 0]$

<u>Alternatively</u>
One can also use cross-products to show that $\sin\theta = 1 \Rightarrow \theta = 90^\circ$.

$$\bar{u} \wedge \bar{v} = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ 1 & 2 & 0 \\ -2 & 1 & 0 \end{vmatrix} = 5\sin\theta$$

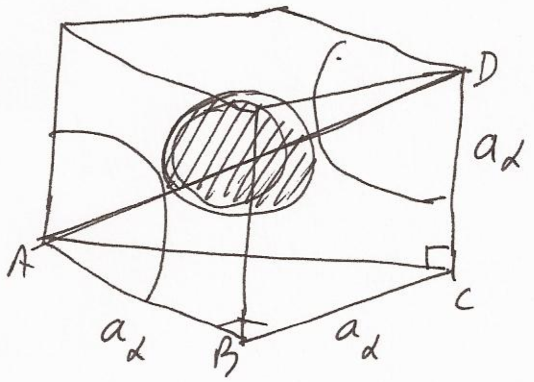
$$\Rightarrow \left|\hat{k}\,(1 - (-2)(2))\right| = 5\sin\theta$$

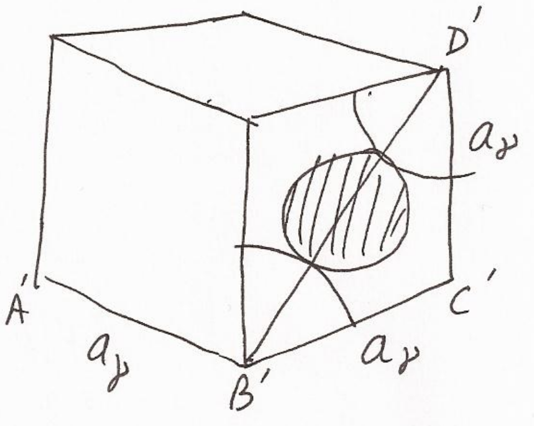
$$\Rightarrow 5 = 5\sin\theta$$

$$\therefore \underline{\theta = 90^\circ}.$$

3. α_{Fe} (BCC) $\qquad$ γ_{Fe} (FCC)

$a_{\alpha} = 0.286\,nm$ $\qquad$ Find a_γ.





$$(AC)^2 = (AB)^2 + (BC)^2$$

$$= 2a_\alpha^2$$

$$(AD)^2 = (AC)^2 + (DC)^2$$

$$= 2a_\alpha^2 + a_\alpha^2$$

$$(AD)^2 = 3a_\alpha^2$$

$AD = a_\alpha\sqrt{3}$ (length of body diagonal)

$= 4r$

(r = radius of iron atom hardball)

$$B'D' = 4r$$

$$(B'D')^2 = (B'C')^2 + (D'C')^2$$

$$= a_\gamma^2 + a_\gamma^2$$

$$(B'D')^2 = 2a_\gamma^2$$

$$B'D' = 4r = a_\gamma\sqrt{2}$$

Therefore

$$a_\alpha\sqrt{3} = a_\gamma\sqrt{2}$$

$$\therefore\ a_\gamma = a_\alpha\sqrt{\frac{3}{2}}$$

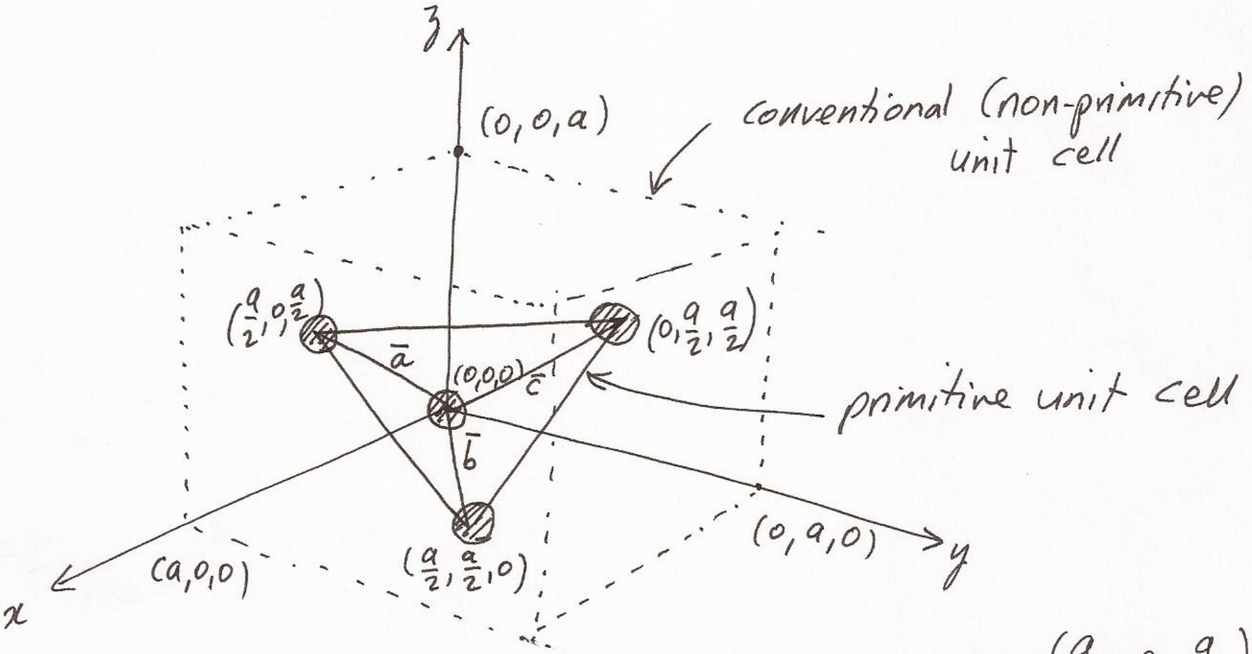
$$= 0.286\sqrt{\frac{3}{2}}\ nm$$

$$= \underline{\underline{0.350\,nm}}$$

4. (i) Primitive unit cell – is the smallest area (in 2-D) or volume (in 3-D) that can generate a lattice by repeated operations of symmetry such as translations, rotations, etc... A Conventional (or non-primitive) unit cell is the equivalent representation that offers convenience of handling rather than minimal area or volume.

(Write in your own words to show understanding rather than just memory).

(ii)



Locate vectors $\bar{a}$, $\bar{b}$ and $\bar{c}$ i.e.

$$\bar{a} = \left(\frac{a}{2}, 0, \frac{a}{2}\right)$$

$$\bar{b} = \left(\frac{a}{2}, \frac{a}{2}, 0\right)$$

$$\bar{c} = \left(0, \frac{a}{2}, \frac{a}{2}\right)$$

Vol. of conventional unit cell $= V_c = a^3$

Vol. of primitive unit cell $= V_p = \bar{a} \cdot (\bar{b} \wedge \bar{c})$

$$\bar{b} \wedge \bar{c} = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ \frac{a}{2} & \frac{a}{2} & 0 \\ 0 & \frac{a}{2} & \frac{a}{2} \end{vmatrix} = \hat{i}\left(\frac{a^2}{4} - 0\right) - \hat{j}\left(\frac{a^2}{4} - 0\right) + \hat{k}\left(\frac{a^2}{4} - 0\right)$$

$$\therefore \bar{b} \wedge \bar{c} = \left(\frac{a^2}{4}, -\frac{a^2}{4}, \frac{a^2}{4}\right) \Rightarrow V_p = \left(\frac{a}{2}, 0, \frac{a}{2}\right) \cdot \left(\frac{a^2}{4}, -\frac{a^2}{4}, \frac{a^2}{4}\right)$$

$$= \frac{a^3}{8} + 0 + \frac{a^3}{8}$$

$$= \frac{a^3}{4}$$

$$\Rightarrow \boxed{V_p = \frac{V_c}{4}} \quad \text{Proved.}$$

5. Orthorhombic $\Rightarrow a \neq b \neq c$, $\alpha = \beta = \gamma = 90°$.

(i)
$$\left.\begin{aligned} \bar{a} &= \bar{a}_1 = 1.25\hat{i} = (1.25, 0, 0) \\ \bar{b} &= \bar{a}_2 = 2.4\hat{j} = (0, 2.4, 0) \\ \bar{c} &= \bar{a}_3 = 2.0\hat{k} = (0, 0, 2.0) \end{aligned}\right\} \text{Real lattice}$$

$$\therefore V_c = \bar{a} \cdot (\bar{b} \wedge \bar{c}) = \bar{a}_1 \cdot (\bar{a}_2 \wedge \bar{a}_3) = (1.25, 0, 0) \cdot (4.8, 0, 0)$$
$$= \underline{\underline{6\ \text{Å}^3}}$$

(ii) To find the reciprocal lattice there are two possible methods:

Method 1

Since orthorhombic, use

$$\bar{b}_i \cdot \bar{a}_j = 2\pi \delta_{ij}, \quad b_i \angle \bar{a}_i = 0°$$

$$\therefore \bar{b}_1 \cdot \bar{a}_1 = b_1 a_1 \cos 0° = b_1 a_1 = 2\pi$$

Similarly $b_2 a_2 = 2\pi$ and

$b_3 a_3 = 2\pi$

$$\Rightarrow \bar{G} = (\bar{b}_1, \bar{b}_2, \bar{b}_3)$$

$$\left.\begin{aligned} \bar{b}_1 &= b_1 \hat{i} = \frac{2\pi}{a_1}\hat{i} = 5.03\hat{i} \\ \bar{b}_2 &= b_2 \hat{j} = \frac{2\pi}{a_2}\hat{j} = 2.62\hat{j} \\ \bar{b}_3 &= b_3 \hat{k} = \frac{2\pi}{a_3}\hat{k} = 3.14\hat{k} \end{aligned}\right\} \begin{aligned} V_{recip} &= b_1 b_2 b_3 \\ &= 41.38\ \text{Å}^3 \end{aligned}$$

Method 2 (more general)

$$\bar{b}_1 = \frac{2\pi}{V_c}(\bar{a}_2 \wedge \bar{a}_3) = \frac{2\pi}{6}(4.8)\hat{i}$$
$$= 5.03\hat{i}$$

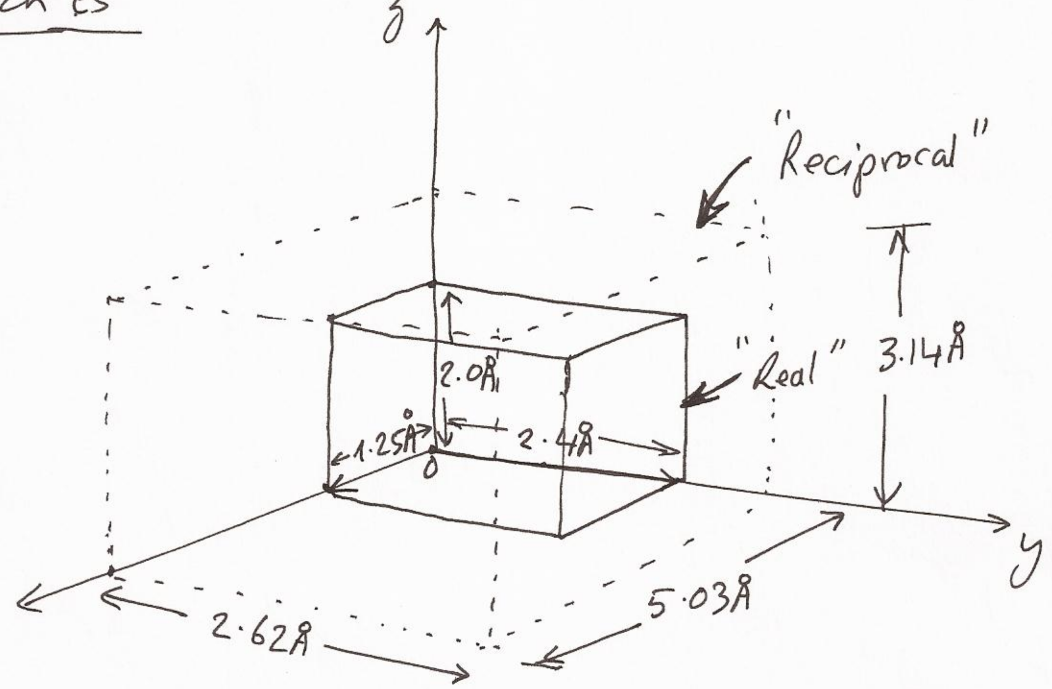
$$\bar{b}_2 = \frac{2\pi}{V_c}(\bar{a}_3 \wedge \bar{a}_1) = \frac{2\pi}{6}(2.5)\hat{j}$$
$$= 2.62\hat{j}$$

$$\bar{b}_3 = \frac{2\pi}{V_c}(\bar{a}_1 \wedge \bar{a}_2) = \frac{2\pi}{6}(3)\hat{k}$$
$$= 3.14\hat{k}$$

$$V_{recip} = \bar{b}_1 \cdot (\bar{b}_2 \wedge \bar{b}_3)$$
$$= 41.38\ \text{Å}^3$$

Hence $\frac{V_{real}}{V^*_{recip.}} = \frac{6}{41.38} \simeq \underline{\underline{0.145}}$.

<u>Sketches</u>



<u>6.</u> See the text book (study guide), set $a = 1$.

$$\Rightarrow \quad X = p = (m-3) + 2\cos\alpha$$

$$\Rightarrow \quad \cos\alpha = \frac{3+(p-m)}{2}$$

and $\quad -1 \leq \cos\alpha \leq 1$

$$\Rightarrow \quad -1 \leq \frac{3+(p-m)}{2} \quad \text{and} \quad \frac{3+(p-m)}{2} \leq 1$$

$$\Rightarrow \quad -5 \leq (p-m) \quad \text{and} \quad (p-m) \leq -1$$

where if p, m are integers then $(p-m)$ is an integer

$$\therefore \quad (p-m) = \{-5, -4, -3, -2, -1\}$$

$$\Rightarrow \quad \alpha = \left\{\pi, \frac{2\pi}{3}, \frac{\pi}{2}, \frac{\pi}{3}, 2\pi\right\}.$$

Section B:

7. $n\lambda = 2d\sin\theta$ where d = separation of (111) planes.

For first-order reflections, $n = 1$

$$\Rightarrow \quad d = \frac{\lambda}{2\sin\theta} = \frac{1.54}{2\sin 19.2^\circ}\,\text{Å} = 2.341\,\text{Å}.$$

The lattice parameter a can be found from

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

$$= 2.341\sqrt{3}\ \text{Å}$$

$$= \underline{\underline{4.055\,\text{Å}}}.$$

In FCC, $n = (8 \times \frac{1}{8}) + (6 \times \frac{1}{2}) = 4$ atoms

Mass of unit cell $= 4m_{Al}$ where m_{Al} = mass of Al atom.

Vol. of unit cell $= a^3$

$\therefore$ Density of aluminium = density of unit cell $= \rho$

$$\Rightarrow \quad \rho = \frac{4m_{Al}}{a^3}, \text{ but } m_{Al} = \frac{\text{Molar mass}}{\text{Avogadro's number}} = \frac{M}{N_A}$$

$$\Rightarrow \quad \rho = \frac{4M}{a^3 N_A} \Rightarrow N_A = \frac{4M}{a^3\rho}$$

$(1\,\text{Å} = 10^{-8}\,\text{cm})$

$$= \frac{4 \times 27\text{g}}{(4.055\times10^{-8})^3(\text{cm}^3) \times 2.7\text{g}(\text{cm}^{-3})} \text{ atoms}$$

$$\therefore N_A = \underline{\underline{6.0\times10^{23} \text{ atoms per mol}}}$$

8.) The structure factor for hkl reflections is

$$S_{\bar{G}}(hkl) = \sum_j f_j \, e^{-i2\pi(hx_j + ky_j + lz_j)}$$

Or, in terms of phase angle δ

$$= \sum_j f_j \, e^{-i\delta_j} = \sum_j f_j(\cos\delta_j - i\sin\delta_j)$$

where $\delta_j = 2\pi(hx_j + ky_j + lz_j)$

For FCC, the indicated atoms have fractional coordinates:

$(0,0,0)$, $(\frac{1}{2}, \frac{1}{2}, 0)$, $(\frac{1}{2}, 0, \frac{1}{2})$ and $(0, \frac{1}{2}, \frac{1}{2})$

Hence $\delta_1 = 0$; $\delta_2 = \pi(h+k)$; $\delta_3 = \pi(h+l)$; $\delta_4 = \pi(k+l)$

$\therefore$ Reflections are observed when h, k, l are all even or all odd.

For the BCC structure, the fractional coordinates are $(0,0,0)$ and $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$.

$\Rightarrow \delta_1 = 0$; $\delta_2 = \pi(h+k+l)$

Hence reflections are observed only when $(h+k+l) = 2n$.

9.) $n\lambda = 2d_{20}\sin 47.75°$

$n\lambda = 2d_{1000}\sin 46.60°$

Because of expansion, $d_{1000} > d_{20}$

$$n\lambda = 2 d_{20} \sin 47.75°$$

$$n\lambda = 2 d_{1000} \sin 46.60°$$

$$\therefore\ d_{20} \sin 47.75° = d_{1000} \sin 46.60° \ ; \qquad \frac{d_{1000}}{d_{20}} = \frac{\sin 47.75°}{\sin 46.60°}$$

$$d_{1000} = d_{20} + \alpha \Delta T \, d_{20}$$

$$= d_{20}(1 + \alpha\Delta T)$$

(by definition of linear expansion, where α = coefficient of expansion)

$$\Rightarrow \frac{d_{1000}}{d_{20}} = 1 + \alpha \Delta T$$

$$\Rightarrow 1 + \alpha\Delta T = \frac{\sin 47.75°}{\sin 46.60°}$$

$$\Rightarrow \alpha = \frac{1}{\Delta T}\left[\frac{\sin 47.75°}{\sin 46.60°} - 1\right]$$

$$= \left(\frac{1}{1000 - 20}\right)\left(\frac{\sin 47.75°}{\sin 46.60°} - 1\right)$$

$$\underline{\alpha = 1.916 \times 10^{-5} \,/°C}$$

10\. (a) <u>Laue equations</u>

$$\bar{G} = (v_1 b_1, v_2 b_2, v_3 b_3)$$

$$\bar{a}_1 = (a_1, 0, 0) \ ; \quad \bar{a}_2 = (0, a_2, 0) \ ; \quad \bar{a}_3 = (0, 0, a_3)$$

Then $\bar{a}_1 \cdot \bar{G} = \bar{a}_1 \cdot v_1 \bar{b}_1 = v_1 \bar{a}_1 \cdot \bar{b}_1 = v_1 2\pi\delta_{11} = 2\pi v_1$

Similarly $\bar{a}_2 \cdot \bar{G} = 2\pi v_2$ and $\bar{a}_3 \cdot \bar{G} = 2\pi v_3$.

(b) Ewald construction – see study guide for method. //