

Day-18

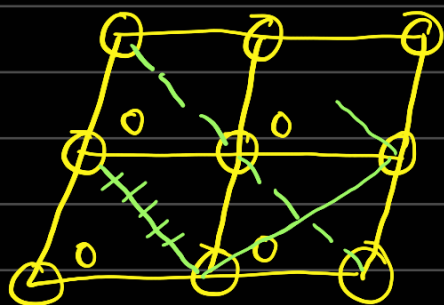
midsem

1) a) 6 atoms per formula unit.

n F.U. associated with a l.p., $n \in \mathbb{Z}$

1 l.p. per w.s. cell $\Rightarrow 6n$ for KCu_3S_2

b)



$P.D_{110} > P.D_{1\bar{1}0}$

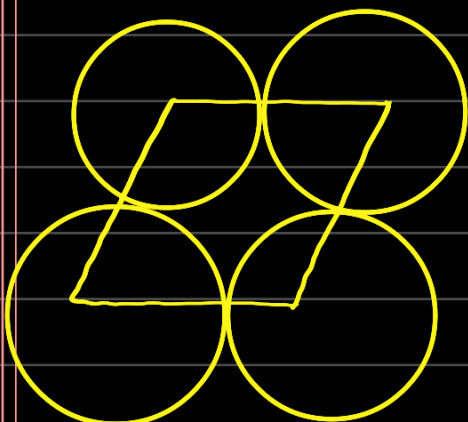
c)

$\left(\frac{1}{3}, \frac{2}{3}, \frac{1}{4}\right) \rightarrow \text{o.v.}$

\downarrow

$[4 \ 8 \ 3]$

d)



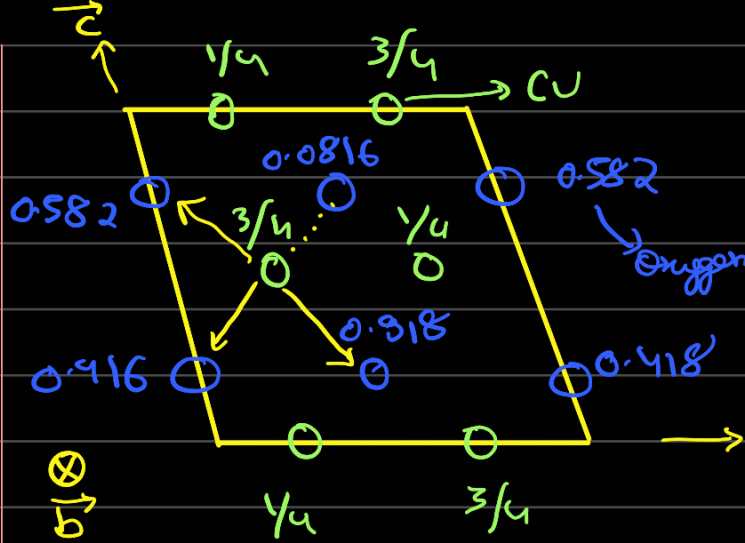
a.p.f $\sim 90\%$

e)

$\text{O} \rightarrow 4, \text{Al} \rightarrow \frac{1}{2} \times 4, \text{Mg} \rightarrow \frac{1}{8} \times 4 + \frac{1}{8} \times 4$

So $\text{Mg Al}_2\text{O}_4$

3.) a.)



$$Cu: \left(\frac{1}{2}, \frac{1}{2}, 0\right),$$

$$\left(\frac{1}{2}, \frac{1}{2}, 1\right)$$

$$MC: \left(\frac{1}{2}, \frac{1}{2}, 0\right)$$

$$\left(\frac{3}{4}, \frac{3}{4}, 0\right),$$

$$\left(\frac{3}{4}, \frac{3}{4}, 1\right)$$

$$\left(, 1.0816, \right)$$

$$\left(\frac{1}{4}, \frac{3}{4}, \frac{1}{2}\right)$$

$$\left(\frac{3}{4}, \frac{1}{4}, \frac{1}{2}\right)$$

$$\left(\frac{3}{4}, \frac{1}{4}, \frac{1}{2}\right)$$

$$O: \left(0, 0.482, \frac{1}{4}\right),$$

$$\left(1, 0.482, \frac{1}{4}\right)$$

$$\left(\frac{1}{2}, 0.9182, \frac{1}{4}\right)$$

$$\left(0, 0.5816, \frac{3}{4}\right), \left(1, 0.5816, \frac{3}{4}\right)$$

$$\left(\frac{1}{2}, 0.0816, \frac{3}{4}\right)$$

b.) i.)

$$\left(\frac{1}{4}, \frac{3}{4}, \frac{1}{2}\right)$$

ii.)

4 O atoms in coordination to Cu.

iii.)

$$g_{ij} = \begin{bmatrix} a^2 & 0 & ac \cos \gamma \\ 0 & b^2 & 0 \\ ac \cos \gamma & 0 & c^2 \end{bmatrix}$$

$$\left(\frac{1}{4}, \frac{3}{4}, \frac{1}{2}\right) \text{ to } \left(0, 0.4182, \frac{1}{4}\right)$$

$$B1 = \left[\frac{1}{4} \quad 0.3318 \quad \frac{1}{4}\right]$$

$$\sqrt{B_i g_{ij} B_j} \simeq 1.95 \text{ \AA}$$

$$\text{iii)} \quad 180^\circ, 95.719, 180^\circ - 95.719^\circ$$

c) i) let $[u \ v \ w]$ be zone-axis.

$$\text{so } hu + kv + lw = 0$$

$$\text{put } [00\bar{2}] \Rightarrow w = 0$$

$$\text{put } [110] \Rightarrow u + v = 0$$

$$\text{so } [u \ -u \ 0] \equiv [1 \ \bar{1} \ 0]$$

ii) let normal axis $\rightarrow [u \ v \ w]$

$$\text{so } [u \ v \ w] \cdot [1 \ \bar{1} \ 0] = 0$$

$$\Rightarrow [u \ v \ w] g_{ij} \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix} = 0$$

and $\angle \phi$ with black dotted line

$$\text{Now, } \frac{[u \ v \ w] \cdot [\bar{1} \ \bar{1} \ 0]}{|t_{uvw}| \times \frac{1}{d_{\bar{1}\bar{1}0}}} = \cos \phi$$

$$\Rightarrow \frac{-(u+v) d_{\bar{1}\bar{1}0}}{|t_{uvw}|} = \cos \phi$$

$$\text{And } \frac{-2w \cdot d_{00\bar{2}}}{|t_{uvw}|} = \cos \theta$$

$$\text{so } \frac{\cos \phi}{\cos \theta} = \frac{(v+v)}{2w} \frac{d_{110}}{d_{002}}$$

$$w \approx G(v+v) \quad (G \in \mathbb{I})$$

2.) a) atoms at vertices and body centre.
But not cI as not same atom there.

so all (hkl) possible

$(100), (110), (111) \rightarrow 1^{\text{st}} 3 \text{ reflection}$

b) $2\theta \rightarrow 11, 15.5, 19, 22.1, 24.7, 27$

$$d = \frac{\lambda}{2 \sin \theta} : 8.036, 5.712, 4.666, 4.013, 3.601, 3.299$$

$$\sqrt{h^2 + k^2 + l^2} : 1, \sqrt{2}, \sqrt{3}, 2, \sqrt{5}, \sqrt{6}$$

$$a_{\text{avg}} = 8.061 \text{ \AA}$$

$$h^2 + k^2 + l^2 \text{ ratio} = 1 : 2 : 3 : 4 : 5 : 6$$

$(110), (200), (211), (220), (310), (222)$

c) cF $\rightarrow (111, \cancel{200}, 311, 220) \rightarrow (400)$

But,

_____	1
_____	3/4
_____	1/2
_____	1/4
_____	0

