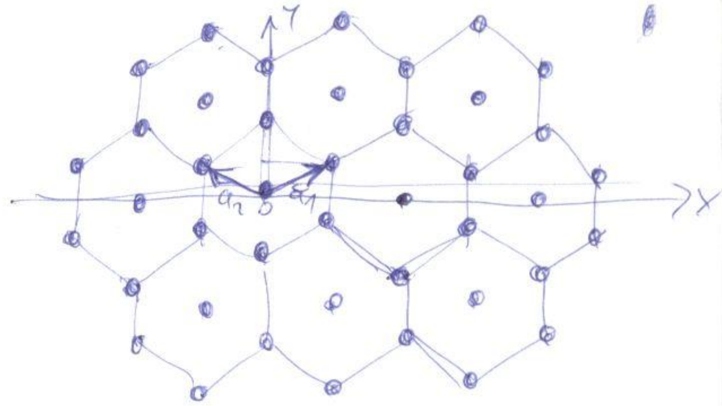
/ Zad2



a) $\bar{a}_1 = \frac{\sqrt{3}}{2} a \bar{e}_x + \frac{1}{2} a \bar{e}_y$

$\bar{a}_2 = -\frac{\sqrt{3}}{2} a \bar{e}_x + \frac{1}{2} a \bar{e}_y$

$\bar{a}_3 = c \bar{e}_z$

$$d_{hkl} = \frac{2\pi}{|\bar{G}_{hkl}|} \qquad \bar{G}_{hkl} = h\bar{\rho}_1 + k\bar{\rho}_2 + l\bar{\rho}_3$$

$$\bar{a}_i \circ \bar{\rho}_j = 2\pi \delta_{ij} \quad , \quad V = \bar{a}_1 \circ (\bar{a}_2 \times \bar{a}_3)$$

$$\bar{\rho}_1 = \frac{2\pi}{V} \bar{a}_2 \times \bar{a}_3 \quad , \quad \bar{\rho}_2 = \frac{2\pi}{V} \bar{a}_3 \times \bar{a}_1 \, , \quad \bar{\rho}_3 = \frac{2\pi}{V} \cdot \bar{a}_1 \times \bar{a}_2$$

$$\bar{a}_2 \times \bar{a}_3 = \begin{vmatrix} \bar{e}_x & \bar{e}_y & \bar{e}_z \\ -\frac{\sqrt{3}}{2}a & \frac{1}{2}a & 0 \\ 0 & 0 & c \end{vmatrix} = \bar{e}_x \frac{1}{2}ac + \frac{\sqrt{3}}{2} ac \bar{e}_y$$

$$V = \bar{a}_1 \circ (\bar{a}_2 \times \bar{a}_3) = \frac{\sqrt{3}}{2} a \cdot \frac{1}{2} ac + \frac{1}{2} a \cdot \frac{\sqrt{3}}{2} ac = \frac{\sqrt{3}}{2} a^2 c$$

$$\bar{a}_3 \times \bar{a}_1 = \begin{vmatrix} \bar{e}_x & \bar{e}_y & \bar{e}_z \\ 0 & 0 & c \\ \frac{\sqrt{3}}{2}a & \frac{1}{2}a & 0 \end{vmatrix} = \bar{e}_x \left(-\frac{1}{2}ac\right) + \bar{e}_y \frac{\sqrt{3}}{2} ac$$

$$\bar{a}_1 \times \bar{a}_2 = \begin{vmatrix} \bar{e}_x & \bar{e}_y & \bar{e}_z \\ \frac{\sqrt{3}}{2}a & \frac{1}{2}a & 0 \\ -\frac{\sqrt{3}}{2}a & \frac{1}{2}a & 0 \end{vmatrix} = \bar{e}_z \left(\frac{\sqrt{3}}{4}a^2 + \frac{\sqrt{3}}{4}a^2\right) = \bar{e}_z \frac{\sqrt{3}}{2} a^2$$

$$\bar{\rho}_1 = \frac{2\pi}{\frac{\sqrt{3}}{\cancel{2}} a \cancel{c}} \cdot \left(\bar{e}_x \cdot \frac{1}{\cancel{2}} \cancel{ac} + \bar{e}_y \frac{\sqrt{3}}{\cancel{2}} \cancel{ac}\right) = \frac{2\pi}{a} \cdot \left(\bar{e}_x \frac{\sqrt{3}}{3} + \bar{e}_y 1\right)$$

$$\bar{\rho}_2 = \frac{2\pi}{\frac{\sqrt{3}}{\cancel{2}} a \cancel{c}} \cdot \left(\bar{e}_x \cdot \left(-\frac{1}{\cancel{2}} \cancel{ac}\right) + \bar{e}_y \frac{\sqrt{3}}{\cancel{2}} \cancel{ac}\right) = \frac{2\pi}{a} \cdot \left(\bar{e}_x \left(-\frac{\sqrt{3}}{3}\right) + \bar{e}_y 1\right)$$

$$\bar{\rho}_3 = \frac{2\pi}{\frac{\sqrt{3}}{2} a^2 c} \cdot \bar{e}_z \frac{\sqrt{3}}{2} a^2 = \frac{2\pi}{c} \cdot \bar{e}_z$$

$$\bar{G}_{hkl} = h\cdot \frac{2\pi}{a}\left(\bar{e}_x \frac{\sqrt{3}}{3} + \bar{e}_y\cdot 1\right) + k\,\frac{2\pi}{a}\cdot\left(\bar{e}_x\left(-\frac{\sqrt{3}}{3}\right) + \bar{e}_y 1\right) + \frac{2\pi}{c}\cdot \bar{e}_z\cdot l =$$

$$= \bar{e}_x\left(\frac{2\pi}{a}\cdot\frac{\sqrt{3}}{3}h - \frac{2\pi}{a}\cdot\frac{\sqrt{3}}{3}\cdot k\right) + \bar{e}_y\left(\frac{2\pi}{a}\cdot h + \frac{2\pi}{a}k\right) + \vec{e}_z\ \frac{2\pi}{c}\cdot l$$

$$|\bar{G}_{hkl}| = \sqrt{\left(\frac{2\pi}{a}\cdot\frac{\sqrt{3}}{3}\right)^2(h-k)^2 + \left(\frac{2\pi}{a}\right)^2\cdot(h+k)^2 + \left(\frac{2\pi}{c}\right)^2\cdot l^2}$$

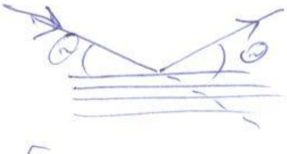
$$d_{hkl} = \frac{2\pi}{|\bar{G}_{hkl}|} = \frac{1}{\sqrt{\frac{(h-k)^2}{3a^2} + \frac{(h+k)^2}{a^2} + \frac{l^2}{c^2}}} =$$

$$= \frac{1}{\sqrt{\frac{h^2-2hk+k^2}{3a^2} + \frac{h^2+2hk+k^2}{a^2} + \frac{l^2}{c^2}}} =$$

7 pkt

$$= \frac{1}{\sqrt{\frac{4h^2}{3a^2} + \frac{4k^2}{3a^2} + \frac{4kh}{3a^2} + \frac{l^2}{c^2}}} = \frac{1}{\sqrt{\frac{4}{3a^2}\cdot(h^2+k^2+kh) + \frac{l^2}{c^2}}}$$

b) $2d\sin\Theta = n\lambda$



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$$d_{100} = \frac{1}{\sqrt{\frac{4}{3a^2}\cdot 1}} = \frac{\sqrt{3}a}{2}$$

$$\sin\Theta_{100} = \frac{n\lambda}{2d_{100}} = n\cdot\frac{\lambda}{2\cdot\frac{\sqrt{3}a}{2}} = n\cdot\frac{1.5418\,\text{Å}}{\underbrace{\sqrt{3}}_{1.73\ldots}\cdot 2} \simeq 0.45$$

$$\Theta_{100} \simeq 26.5^\circ$$