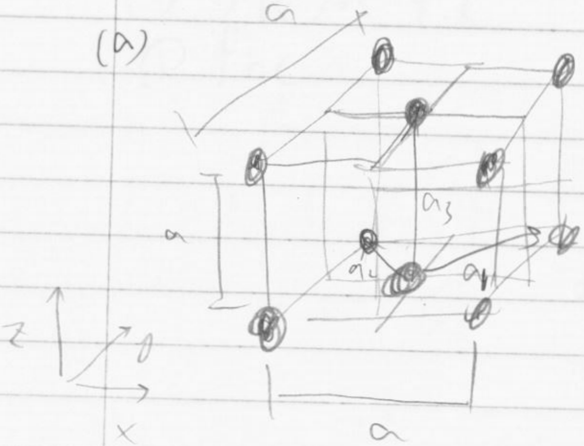
(1) A&M 4.1

(a)



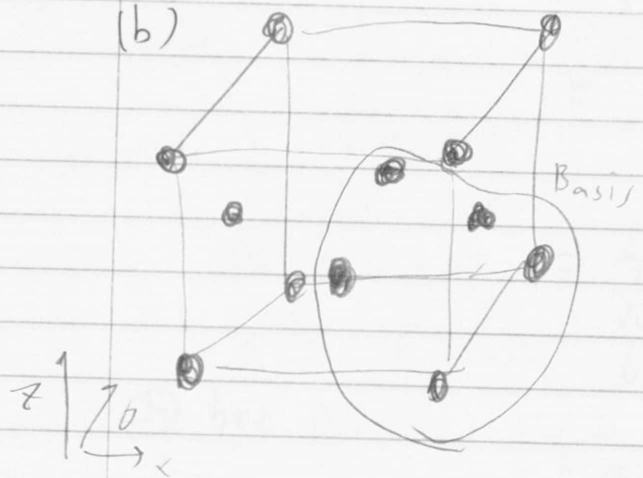
Yes, it is Bravais lattice

$\vec{a}_1 = \left(\frac{a}{2}, \frac{a}{2}, 0\right)$

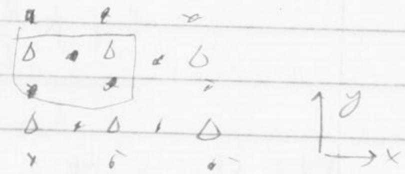
$\vec{a}_2 = \left(\frac{-a}{2}, \frac{a}{2}, 0\right)$

$\vec{a}_3 = (0, 0, a)$

(b)



No, no Bravais lattice



Basis : 5 - points

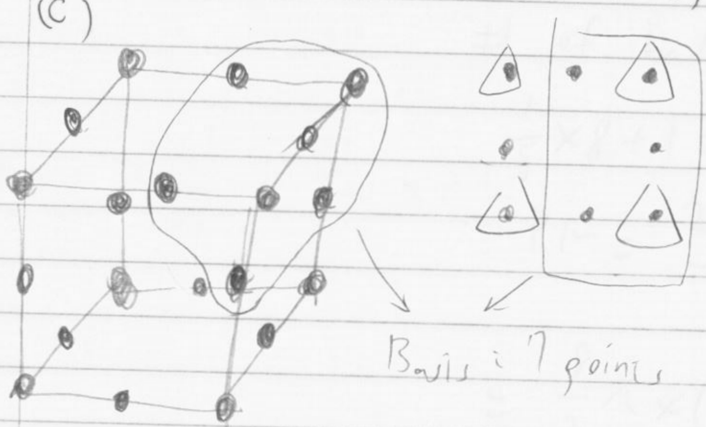
$\vec{a}_1 = (a, 0, 0)$

$\vec{a}_2 = (0, a, 0)$

$\vec{a}_3 = (0, 0, a)$

(c)

No, no Bravais



Basis : 7 points

Basis : 7 - points

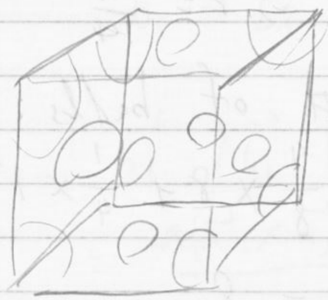
$\vec{a}_1 = (a, 0, 0)$

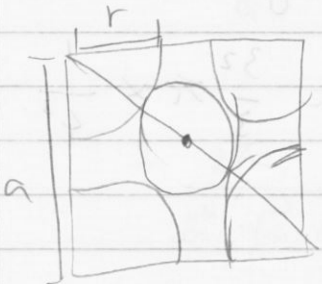
$\vec{a}_2 = (0, a, 0)$

$\vec{a}_3 = (0, 0, a)$

(2) A&M 4.6

① fcc





$4r = a \cdot \sqrt{2}$

$\Rightarrow r = \frac{\sqrt{2}}{4} a$

# of balls in unit cell:

$\frac{1}{8} \times 8 + \frac{1}{2} \times 6 = 1 + 3 = 4$

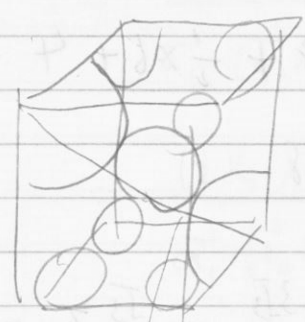
$\therefore$ packing fraction (PF)

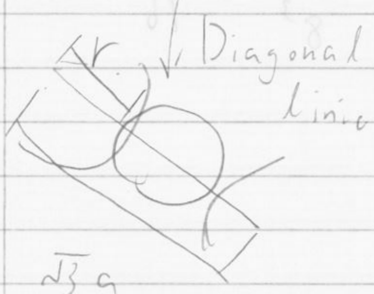
$$= \frac{4 \times \frac{4}{3} \pi r^3}{a^3}$$

$$= \frac{16}{3} \pi \times \left(\frac{\sqrt{2}}{4}\right)^3 = \frac{16}{3} \times \frac{2\sqrt{2}}{64} \pi$$

$$= \frac{\sqrt{2}}{6} \pi = 0.74$$

② bcc





$4r = a \cdot \sqrt{3}$

$\Rightarrow r = \frac{\sqrt{3}}{4} a$

# of balls in unit cell:

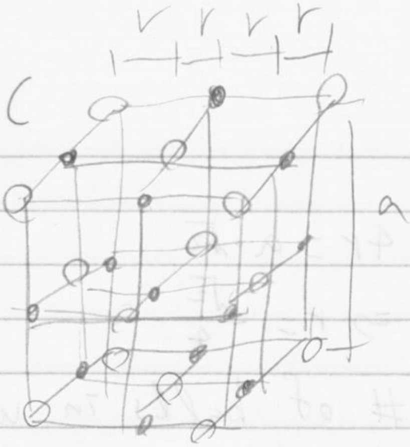
$\frac{1}{8} \times 8 + 1 = 2$

$$\therefore PF = \frac{2 \times \frac{4}{3} \pi r^3}{a^3}$$

$$= \frac{8}{3} \pi \times \left(\frac{\sqrt{3}}{4}\right)^3 = \frac{\sqrt{3}\,\pi}{8} = 0.68$$

SC

③



$4r = a$

$\Rightarrow r = \frac{a}{4}$

\# of balls:

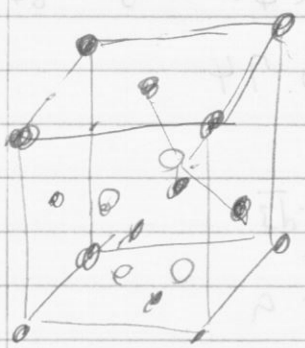
$\frac{1}{8} \times 8 + \frac{1}{4} \times 12 + \frac{1}{2} \times 6 + 1$

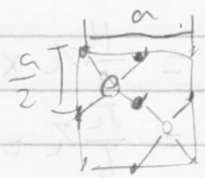
$= 8$

$\therefore PF = \frac{\frac{4}{3}\pi r^3 \times 8}{a^3} = \frac{32}{3}\pi \times \frac{1}{4^3} = \frac{\pi}{6}$

$= 0.52$

④ Diamond





$4r = \frac{a}{2} \cdot \sqrt{3}$

$\Rightarrow r = \frac{\sqrt{3}}{8} a$

\# of balls:

$\frac{1}{8} \times 8 + \frac{1}{2} \times 6 + 4 = 8$

$PF = \frac{\frac{4}{3}\pi r^3 \times 8}{a^3}$

$= \frac{32}{3}\pi \times \frac{3\sqrt{3}}{8^3} = \frac{\sqrt{3}}{16}\pi = 0.34$

(3) A&M 5.1

(a)

$$b_1 = 2\pi \frac{\vec{a_2} \times \vec{a_3}}{\vec{a_1} \cdot (\vec{a_2} \times \vec{a_3})}$$

$$\vec{b_1} \cdot (\vec{b_2} \times \vec{b_3})$$

$$= \frac{2\pi(\vec{a_2} \times \vec{a_3})}{\vec{a_1} \cdot (\vec{a_2} \times \vec{a_3})} \cdot (\vec{b_2} \times \vec{b_3})$$

$$= \frac{2\pi}{\vec{a_1} \cdot (\vec{a_2} \times \vec{a_3})} \vec{b_2} \cdot \left[\vec{b_3} \times (\vec{a_2} \times \vec{a_3})\right]$$

$$= \frac{2\pi}{\vec{a_1} \cdot (\vec{a_2} \times \vec{a_3})} \vec{b_2} \cdot \left[\vec{a_2}\,(\vec{a_3} \cdot \vec{b_3}) - \vec{a_3}\,(\vec{a_2} \cdot \vec{b_3})\right]$$

$$= \frac{2\pi}{\vec{a_1} \cdot (\vec{a_2} \times \vec{a_3})} (\vec{a_2} \cdot \vec{b_2})(\vec{a_3} \cdot \vec{b_3})$$

$$(\because \vec{a_i} \cdot \vec{b_j} = 2\pi\delta_{ij})$$

$$= \frac{(2\pi)^3}{\vec{a_1} \cdot (\vec{a_2} \times \vec{a_3})}$$

(b)

$$2\pi \frac{\vec{b}_2 \times \vec{b}_3}{\vec{b}_1 \cdot (\vec{b}_2 \times \vec{b}_3)}$$

$$= 2\pi \frac{\vec{b}_2 \times \vec{b}_3}{\frac{(2\pi)^3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}} = \frac{1}{(2\pi)^2} V_a \, (\vec{b}_2 \times \vec{b}_3)$$

$$\left(V_a := \vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3) \right)$$

$$= \frac{1}{(2\pi)^2} V_a \, \vec{b}_2 \times \left(2\pi \frac{\vec{a}_1 \times \vec{a}_2}{\vec{a}_3 \cdot (\vec{a}_1 \times \vec{a}_2)} \right)$$

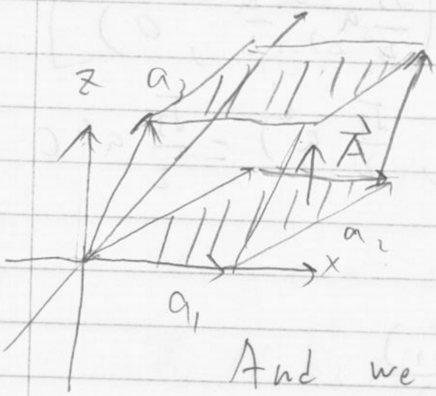
$$= \frac{1}{2\pi} \cdot \left[\vec{b}_2 \times (\vec{a}_1 \times \vec{a}_2) \right]$$

$$= \frac{1}{2\pi} \cdot \left[\vec{a}_1 (\vec{a}_2 \cdot \vec{b}_2) - \vec{a}_2 (\vec{a}_1 \cdot \vec{b}_2) \right]$$

$$= \vec{a}_1$$

(c)

Without loss of generality, let's assume that $\vec{a}_1, \vec{a}_2$ lie on the x, y plane, and $\vec{a}_1 // \hat{x}$



We know from the property of the outer product that

$\vec{A} := \vec{a}_1 \times \vec{a}_2 \; // \; +\hat{z}$

$|\vec{A}|$ = Area of parallelogram expanded by $\vec{a}_1, \vec{a}_2$.

And we also know that

V (Volume of primitive cell)

$= |\vec{A}| \times h$ (height of the primitive cell)

h = z component of $\vec{a}_3$

$= |\vec{a}_3 \cdot \hat{z}|$

$= \dfrac{|\vec{a}_3 \cdot \vec{A}|}{|\vec{A}|}$

$\therefore V = |\vec{a}_3 \cdot \vec{A}| = |\vec{a}_3 \cdot (\vec{a}_1 \times \vec{a}_2)|$.

(4)

(a)

$$V = \vec{a}_3 \cdot (\vec{a}_1 \times \vec{a}_2)$$

$$= (0, 0, c) \cdot \left[\left(\frac{\sqrt{3}}{2} a, \frac{a}{2}, 0 \right) \times \left(\frac{-\sqrt{3}}{2} a, \frac{a}{2}, 0 \right) \right]$$

$$= (0, 0, c) \cdot \left(0, 0, \frac{\sqrt{3}}{2} a^2 \right) = \frac{\sqrt{3}}{2} a^2 c$$

$=$

(b) $$\vec{b}_1 = 2\pi \cdot \frac{(\vec{a}_2 \times \vec{a}_3)}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$$

$$= 2\pi \cdot \frac{\left(-\frac{\sqrt{3}}{2} a, \frac{a}{2}, 0\right) \times (0, 0, c)}{\frac{\sqrt{3}}{2} a^2 c}$$

$$= \frac{4\pi}{\sqrt{3} a^2 c} \left(\frac{ac}{2}, \frac{\sqrt{3}}{2} ac, 0 \right)$$

$$= \left(\frac{2\pi}{\sqrt{3} a}, \frac{2\pi}{a}, 0 \right)$$

$$\vec{b}_2 = 2\pi \cdot \frac{(\vec{a}_3 \times \vec{a}_1)}{\vec{a}_2 \cdot (\vec{a}_3 \times \vec{a}_1)}$$

$$= \frac{4\pi}{\sqrt{3} a^2 c} \left(-\frac{ac}{2}, \frac{\sqrt{3}}{2} ac, 0 \right)$$

$$= \left(-\frac{2\pi}{\sqrt{3} a}, \frac{2\pi}{a}, 0 \right)$$

$$\vec{b}_3 = \frac{2\pi\,(\vec{a}_1 \times \vec{a}_2)}{\vec{a}_3 \cdot (\vec{a}_1 \times \vec{a}_2)}$$

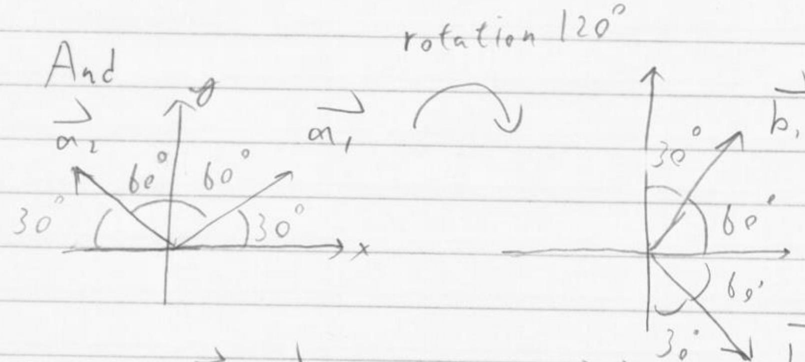
$$= \frac{4\pi}{\sqrt{3}\,a^2 c} \cdot \left(0,\ 0,\ \frac{\sqrt{3}}{2} a^2\right)$$

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

We can see that

$\vec{a}_3 \,//\, \vec{b}_3 \,//\, \hat{z}$

And



$\vec{a}_1, \vec{a}_2 \longrightarrow \vec{b}_1, \vec{b}_2$

$\Rightarrow$ Also hexagonal lattice

(c)

1st Brillouin