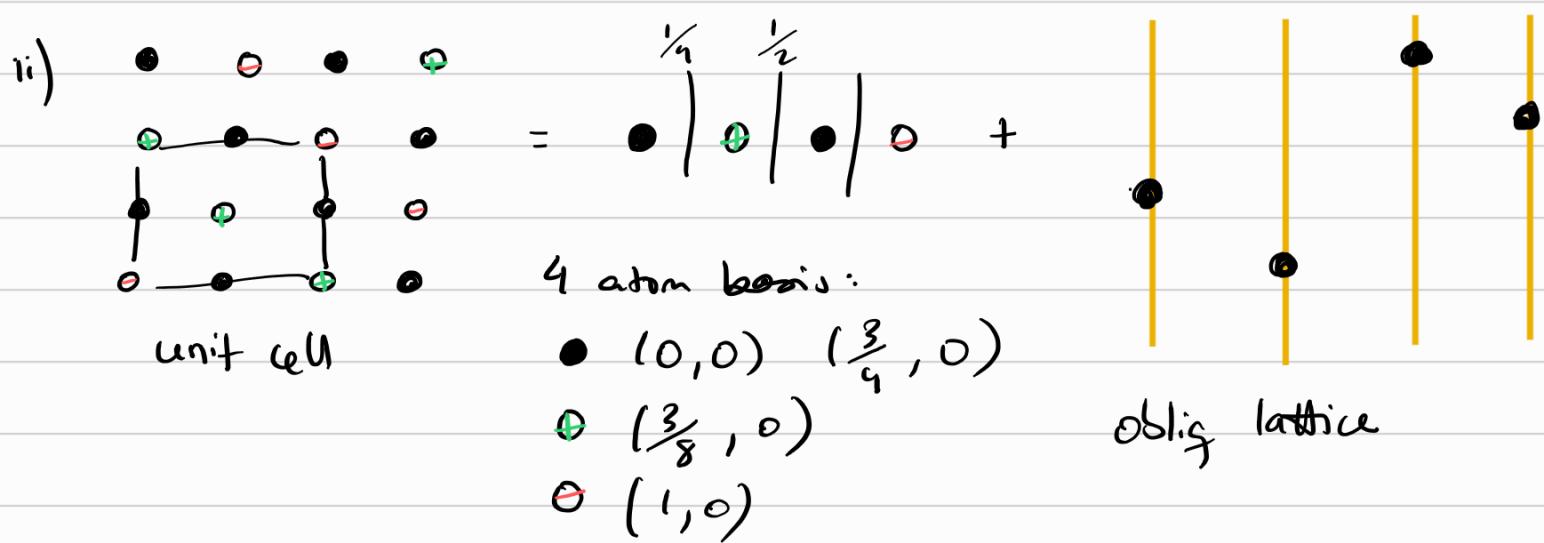


3 atom basis:

- $\bullet (0,0)$
- $\circ (1,0), (0,1)$



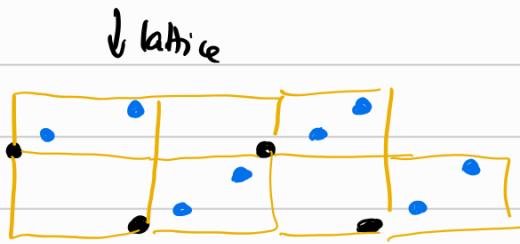
2) $\vec{a} = \left(\frac{\sqrt{3}a}{2}\right)\vec{i} + \frac{a}{2}\vec{j}$

$\vec{b} = \frac{\sqrt{3}a}{2}\vec{i} - \frac{a}{2}\vec{j}$

basis $(u, v) = \left(\frac{1}{3}, \frac{1}{3}\right) \quad \mathcal{E} \left(\frac{2}{3}, \frac{2}{3}\right)$



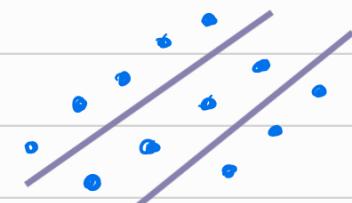
$\xrightarrow{\text{copy}}$



hexagonal
mirror planes

rotations $60^\circ, 120^\circ, 180^\circ, \dots$

no 180° symmetry



Weigner cell:



3) \approx not in the mood



a) $R_{nn} = \frac{\sqrt{3}a}{2} \rightarrow \text{atomic rad} = \frac{\sqrt{3}a}{4}$ ✓

b) $V_{\text{atom}} = \frac{4}{3}\pi r^3 = \frac{4}{3}\pi \frac{8\sqrt{3}a^3}{4^3} = \frac{\sqrt{3}\pi}{4^2} a^3$

$V_{\text{cell}} = a^3$ $\frac{V_{\text{atom}}}{V_{\text{cell}}} = \frac{\sqrt{3}}{16}\pi$

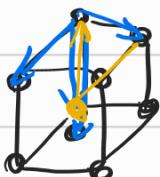
Good A4
guidance

2 atoms bcc $\therefore PF = 2 \times \frac{\sqrt{3}}{16}\pi \approx 0.68$ ✓ ↴

c) $V_{\text{atom}} = \frac{\sqrt{3}}{16}\pi$

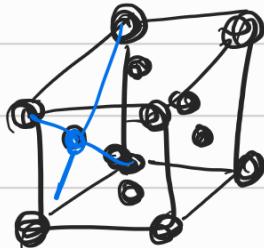
$2 \times V_{\text{atom}} = \frac{\sqrt{3}}{8}\pi$

d)



Coordination $n=4$

ii) fcc



a) $R_{nn} = \frac{a}{\sqrt{2}}$ $r_{\text{atom}} = \frac{a}{2\sqrt{2}}$

b) $V_{\text{atom}} = \frac{4}{3}\pi r^3 = \frac{4}{3}\pi \frac{a^3}{2^4\sqrt{2}}$

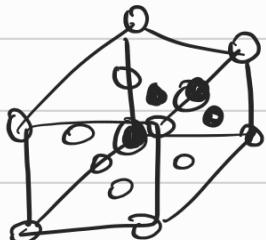
$\frac{V_{\text{atom}}}{V_{\text{cell}}} = \frac{\frac{\pi}{3} \frac{a^3}{4\sqrt{2}}}{a^3} = \frac{\pi}{3 \cdot 4\sqrt{2}}$

$4 \times \frac{V_{\text{atom}}}{V_{\text{cell}}} = \frac{\pi}{3\sqrt{2}} \approx 0.74 = PF$

c) $4 \times V_{\text{atom}} = \frac{\pi a^3}{3\sqrt{2}}$

d) $4 = \text{coord } n=4$

iii)



$$a) R_{nn} = \frac{\sqrt{3}a}{4}, r = \frac{\sqrt{3}}{8}a$$

$$b) V_{at} = \frac{4}{3} \pi r^3 = \frac{4}{3} \pi \frac{8\sqrt{3}}{4 \cdot 8^2} a^3 = \frac{\pi \sqrt{3} a^3}{2 \cdot 8^2}$$

*Diamond
8 atoms
basis*

$$\cancel{9}^8 \times \frac{V_{at}}{U_{\text{cell}}} = \frac{\pi \sqrt{3} a^3}{2 \cdot 8^2} = \frac{\pi \sqrt{3}}{2 \cdot 8^2} \times \cancel{9}^8 \approx 0.384 = \text{PF}$$

$$(c) V_{at} = \frac{\pi \sqrt{3} a^3}{2 \cdot 8^2} \frac{a^3}{z}$$

$$8 \times V_{at} = \frac{\pi \sqrt{3} a^3}{16}$$

$$(d) \text{ coordination number} = 6$$

$$5) \vec{a} = a\vec{i} \quad a = 2.461 \text{ \AA}$$

$$\vec{b} = \frac{a}{2}\vec{i} + \frac{\sqrt{3}a}{2}\vec{j} \quad c = 6.708 \text{ \AA}$$

$$c = c\vec{u}$$

$$\text{at } (u, v, w) = \left(\frac{1}{3}, \frac{1}{3}, 0\right), \left(\frac{2}{3}, \frac{2}{3}, 0\right), \left(\frac{1}{3}, \frac{1}{3}, \frac{1}{2}\right), \left(0, 0, \frac{1}{2}\right)$$

$$\text{density} \approx 2.2 \text{ g/cm}^3$$

$$(i) V = |\vec{a} \cdot (\vec{b} \times \vec{c})| = \left| \begin{vmatrix} a/2 \\ 0 \\ 0 \end{vmatrix} \cdot \left(\begin{vmatrix} a/2 \\ \sqrt{3}a/2 \\ 0 \end{vmatrix} \times \begin{vmatrix} 0 \\ 0 \\ c \end{vmatrix} \right) \right|$$



$$= \left(\begin{vmatrix} a/2 \\ 0 \\ 0 \end{vmatrix} \cdot \begin{vmatrix} \vec{i} & \vec{j} & \vec{u} \\ a/2 & \sqrt{3}a/2 & 0 \\ 0 & 0 & c \end{vmatrix} \right)$$

$$= \left(\begin{vmatrix} a/2 \\ 0 \\ 0 \end{vmatrix} \cdot \begin{pmatrix} \frac{\sqrt{3}a}{2}c \\ \frac{a}{2}c \\ 0 \end{pmatrix} \right)$$

$$= \frac{\sqrt{3}a^2}{4}c + \frac{a^2}{4}c$$

redo

$$= \frac{a^2}{4} c (\sqrt{3} + 1)$$

$$V \approx 27.73 \text{ } \text{Å}^3$$

35.18

ii) 14.4 g $1 \text{ } \text{Å} = 10^{-10} \text{ m}$
 density = $\frac{\text{weight}}{\text{vol}} = \frac{2.2 \text{ g}}{1 \text{ cm}^3}$

right tech
 wrong n° play

$$\text{weight} = 14.4 \text{ g} \quad \therefore \text{vol} = \frac{14.4}{2.2} = 6.54 \text{ cm}^3$$

$$N^{\circ} \text{ cells} = \frac{\text{Vol pen}}{\text{Vol cell}} = \frac{6.54}{27.73 \times 10^{-9}} \approx 2.36 \times 10^8$$

Atoms/cell = 4 \therefore the pen contains 9.44×10^8 atoms

Realty (i)-(ii)

$$(i) V = |\vec{a} \cdot (\vec{b} \times \vec{c})| = \left| \begin{pmatrix} a_{12} \\ 0 \\ 0 \end{pmatrix} \cdot \left(\begin{pmatrix} a_{12} \\ \sqrt{3}a_{12} \\ 0 \end{pmatrix} \times \begin{pmatrix} 0 \\ 0 \\ c \end{pmatrix} \right) \right|$$

$$\vec{b} \times \vec{c} = \begin{pmatrix} a_{12} \\ \sqrt{3}a_{12} \\ 0 \end{pmatrix} \times \begin{pmatrix} 0 \\ 0 \\ c \end{pmatrix} = \begin{vmatrix} \vec{i} & \vec{j} & \vec{k} \\ a_{12} & \sqrt{3}a_{12} & 0 \\ 0 & 0 & c \end{vmatrix} = \frac{\sqrt{3}a}{2} c \vec{i} - \frac{a}{2} c \vec{j}$$

$$V = \vec{a} \cdot (\vec{b} \times \vec{c}) = \begin{pmatrix} a \\ 0 \\ 0 \end{pmatrix} \cdot \frac{a}{2} c \begin{pmatrix} \sqrt{3} \\ 1 \\ 0 \end{pmatrix} = \frac{a}{2} c (\sqrt{3}a) = \frac{\sqrt{3}a^2 c}{2}$$

$$V \approx \frac{(2.461)^2}{2} 6.708 (\sqrt{3})$$

$$= 35.18 \text{ } \text{Å}^3$$

ii) 14.4 g $1 \text{ } \text{Å} = 10^{-10} \text{ m}$
 density = $\frac{\text{weight}}{\text{vol}} = \frac{2.2 \text{ g}}{1 \text{ cm}^3}$

$$\text{Å} \xrightarrow{10^{-8}} \text{cm}$$

$$\text{Å}^3 \xrightarrow{(10^{-8})^3} \text{cm}^3 \xrightarrow{10^{-24}}$$

$$\text{weight} = 14.4 \text{ g} \quad \therefore \text{vol} = \frac{14.4}{2.2} = 6.54 \text{ cm}^3$$



$$N^{\circ} \text{ cells} = \frac{\text{Vol pen}}{\text{Vol cell}} = \frac{6.54}{35.18 \times 10^{-10}} \approx 1.86 \times 10^{23} \text{ cm}^3$$

Atoms/cell = 4 \therefore the pen contains 7.44×10^{23} atoms

$$(iii) A = \vec{a} \times \vec{b}$$

$$= \begin{vmatrix} \vec{i} & \vec{j} & \vec{u} \\ a & 0 & 0 \\ a/2 & \sqrt{3}a/2 & 0 \end{vmatrix}$$

$$= a^2 \sqrt{3} \frac{\vec{u}}{2}$$

$$= 5.24 \text{ \AA}^2$$

(iv) Carbon

$$A = 5.24 \text{ \AA}^2$$

$$\frac{\text{unit cell}}{7.44 \times 10^{23} \text{ atom}} = 3.72 \times 10^{23} \text{ unit cell}$$

$$\frac{A_{\text{atom}}}{\text{unit cell}} \times \frac{N^{\circ} \text{ atoms}}{\text{unit cells}} = A = 3.72 \times 10^{24} \text{ \AA}^2$$

MAKE SURE U WORK WITH AREAS & VOLS

OF ONLY ATOMS OR ONLY UNIT CELLS

$$v) 1500 \mu\text{m}^2 - 500 \Sigma$$

$$A = 1.95 \times 10^{24} \text{ \AA}^2$$

$$= 1.95 \times 10^{24} \times (10^{-8})^2$$

$$= 1.95 \times 10^8 \text{ cm}^2$$

$$= 1.95 \times 10^{22} \mu\text{m}^2$$

$$\frac{1.95 \times 10^8}{1500 \times 10^{-12}}$$

$$1.95 \times 10^{22} \mu\text{m}^2 - 500$$

$$\frac{1.95 \times 10^{22}}{6.5 \times 10^{22}} = 3$$

6) fcc $a = 3.615 \text{ \AA}$

4 atom basis



$$V = 1 \text{ cm}^3$$

$$V_{\text{fcc}} = \frac{a^3}{4} = 11.81 \text{ \AA}^3$$

$$= 11.81 \times 10^{-24} \text{ cm}^3$$

seem to be doing a
lot of unit conversion mistakes
→ do 1st the following

$$N^{\circ} \text{ fcc cells} = \frac{V_{\text{Cu}}}{V_{\text{fcc}}} = 8.47 \times 10^{22}$$

$$\therefore N^{\circ} \text{ cells} \times \text{Atoms per cell}$$

$$= \text{Atoms in Cu} = 3.39 \times 10^{23}$$

$$\text{Density} = \frac{\text{mass}}{\text{vol}} = \frac{\text{Atoms}}{\text{LCC}}$$

(Na)

$$\text{atomic weight } 23 = 3.818 \times 10^{-26}$$

$$a = 4.23 \text{ \AA}$$

$$\text{Density} = \frac{\text{mass}}{\text{vol}}$$

$$V_{\text{vol}} = \frac{a^3}{2} = \frac{(4.23 \times 10^{-8})^3}{2} = 3.78 \times 10^{-23} \text{ m}^3$$

$$\text{Mass} = N^{\circ} \text{ atoms} \times \text{atomic weight}$$

$$N^{\circ} \text{ atoms bcc cell} = 2$$

$$V_{\text{measured}} = a^3$$

$$N_{\text{cells}} = \frac{V_{\text{measured}}}{V_{\text{bcc}}} = \frac{a^3}{\frac{a^3}{2}} = 2$$

not needed

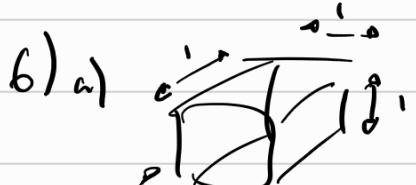
around!

N° atoms = N cells \times atoms per cell
 $= 4$

Mass = $4 \times 3.818 \times 10^{-26} \text{ kg} = 1.53 \times 10^{-25} \text{ kg}$

Wrong
 ↴ see tutorial

PE DO ex ⑥



Fcc 4 atoms / basis

vol fcc = a^3

$V_{\text{struct}} \neq V_{\text{cell}}$
 $\underline{\underline{=}}$
 Vol occ atoms

? $a = 3.615 \text{ \AA}$
 n° atoms

$$\frac{V_{\text{tot}}}{V_{\text{fcc}}} = \frac{(0.01)^3}{(3.615 \times 10^{-10})^3}$$

$$= 2.12 \times 10^{-22} = \frac{n^{\circ}_{\text{fcc}}}{V_{\text{tot}}}$$

Tot at = $\frac{n^{\circ}_{\text{fcc}}}{V_{\text{tot}}} \times \text{f.c. basis} = 8.47 \times 10^{-22}$

b) Atomic weight 23 amu = $3.82 \times 10^{-26} \text{ kg}$

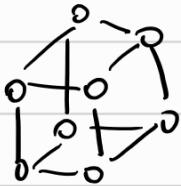
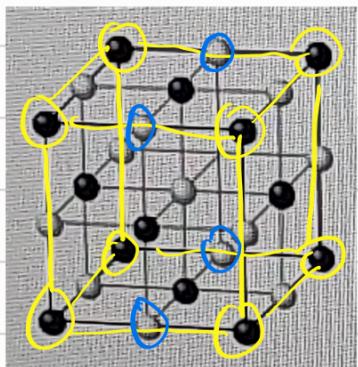
bcc ∵ 2 atoms per basis

$a = 4.23 \text{ \AA}$

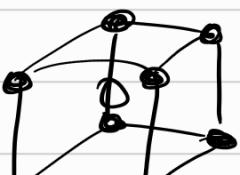
Density = $\frac{\text{mass}}{\text{vol}} = \frac{2 \times 3.82 \times 10^{-26}}{(4.23)^3} = 1.01 \times 10^{-3} \frac{\text{kg}}{\text{m}^3}$

$\cancel{\frac{\text{kg}}{\text{m}^3}}$

7)

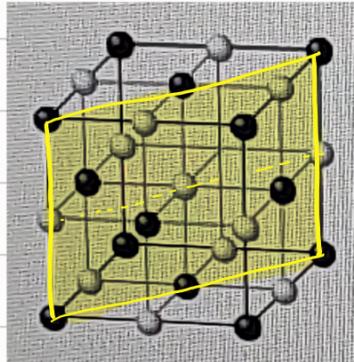


8) Cu

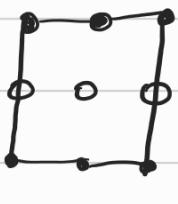


[111] Cl ✓
[210] Cs ✓

9)



2 atom ✓



basis

• 0 +

◦ 0

◦ 0

• (0,0) (½, 0) (1, 0)
◦ (0,1) (½, 1) (1, 1)
◦ (½, 0) (½, ½) (1, ½)

lattice

• • •

◦ • • •

◦ • • •

• (0, 0) rectangles ✓

◦ (0, $\frac{\pi}{4}$)

$\frac{\pi}{2}$

10) [d]

