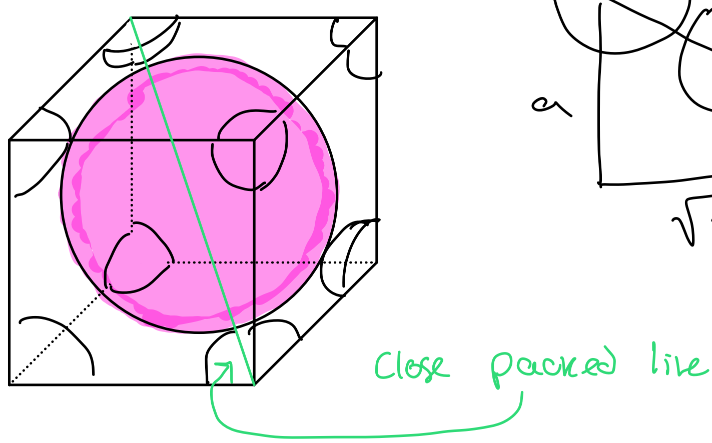
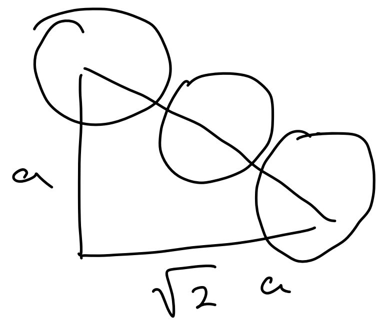
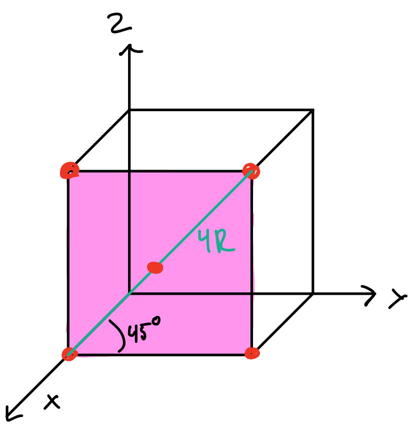
1 BCC radius → volume





$$4r = \sqrt{3}\, a$$
$$a = \frac{4}{\sqrt{3}} r$$
$$V = a^3 = \left[\frac{4}{\sqrt{3}} r\right]^3 = \left[0.1249\ \text{nm} \times \frac{4}{\sqrt{3}}\right]^3$$
$$= 0.02460\ \text{nm}^3$$

2 Planar Density



$\left(1 + 4 \times \frac{1}{4}\right)$ atoms

$$4r \cos 45° = a$$
$$a = 2\sqrt{2}\, r$$
$$A = \left[2\sqrt{2}\, r\right]^2 = 8r^2$$
$$= 0.1242\ \text{nm}^2$$

planar density = $\frac{2 \text{ atoms}}{0.1242 \text{ nm}^2}$ = 16 atoms/nm^2

3 Potassium Iodide

$K^+ \rightarrow 0.138$ nm

$I^- \rightarrow 0.220$ nm

$$\frac{r_{K^+}}{r_{I^-}} = \frac{0.138 \text{nm}}{0.220 \text{nm}} = 0.627$$

predicted to be 6 coordinated → Rock Salt

formula 12.1

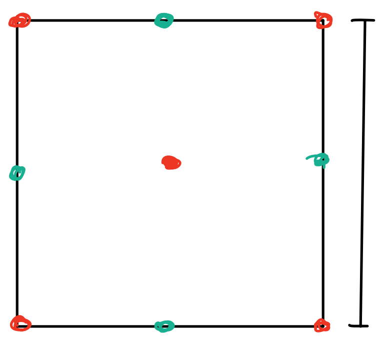
$$\rho = \frac{n'(\Sigma A_c + \Sigma A_A)}{V_c N_A}$$ 14 13

n' is 4 because Rock salt → FCC

$\Sigma A_c = \mu(K) = 39.098$

$\Sigma A_A = \mu(I^-) = 126.904$

looking @ one face



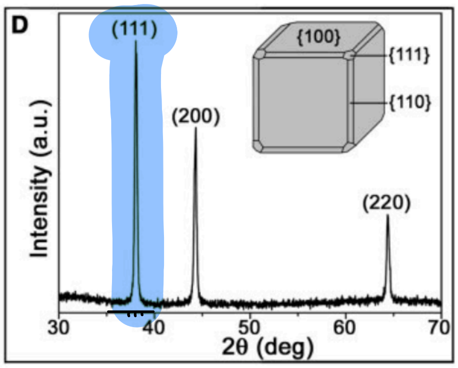
$a = [r_{K^+} + r_I] \times 2 = 0.716$ nm

$$V = a^3 = \left[2(r_K + r_I)\right]^3 = 0.367\ nm^3$$

$$1nm^3 \left(\frac{1\ cm}{10^7\ nm}\right)^3$$

$$\rho = 3.005\ g/cm$$

$\boxed{4}$ wavelength used to replicate plot



$$n\lambda = 2d\sin\theta$$

for (111)

$$d = \frac{a}{\sqrt{1^2+1^2+1^2}} = \frac{a}{\sqrt{3}}$$

go with the value of a they calculated

$$d = \frac{4.088\ \mathring{A}}{\sqrt{3}} = \frac{0.4088\ nm}{\sqrt{3}} = 0.2834\ nm$$

$\sin\theta$ increases as n increases, and over this interval $\sin\theta$ is strictly increasing therefore its fair to assume $n=1$

$$\lambda = 2d\sin\theta$$

2θ looks to me roughly $38°$

plugging in

$$\lambda = 2(0.2834\,nm)\left(\sin\left(\frac{38^\circ}{2}\right)\right)$$
$$= 0.1537\,nm$$

$\boxed{5}$

$\lambda = 0.0711$ $\quad n=1$

a) $\theta = 27^\circ$

$$n\lambda = 2d\sin\theta$$
$$d = \frac{n\lambda}{2\sin\theta} = \frac{(1)(0.0711)}{2\cdot\sin(27/2)} = 0.1523\ nm$$

b

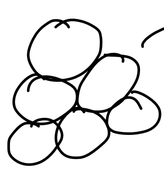
$$d = \frac{a}{\sqrt{3^2+2^2+1^2}} = \frac{a}{\sqrt{14}}$$

$$\Longrightarrow \quad a = \sqrt{14}\, d = 0.5698\ nm$$

for bcc $\quad 4r = \sqrt{3}\,a$

$$r = \frac{\sqrt{3}}{4}a = 0.247\ nm$$

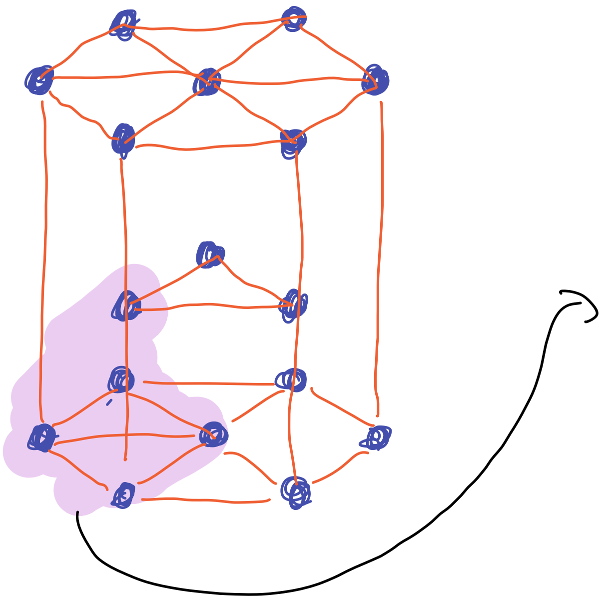
$\boxed{6}$ Show ideal $\frac{c}{a}$ ratio is 1.633



a is clearly 2r

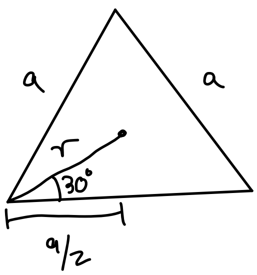
for the close packed planes

now looking from another angle



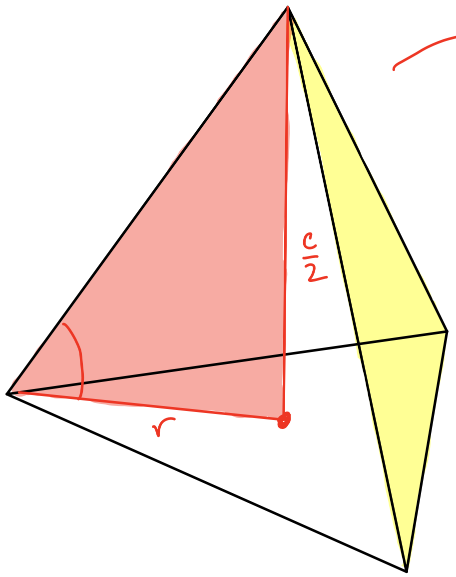
forms triangular pyramid

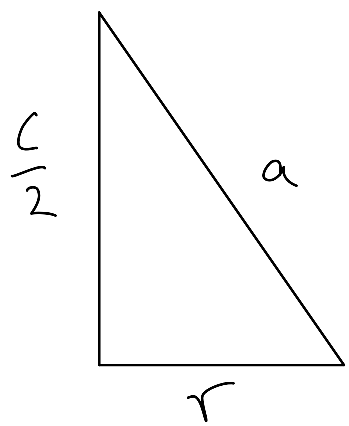
forms a tetrahedron with $h = \frac{1}{2}c$ and base side length a



$$\frac{a}{2} = r\cos 30^\circ$$

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





$$a^2 = r^2 + \left(\frac{c}{2}\right)^2$$

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

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

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

$$\frac{8}{3} = \frac{c^2}{a^2}$$

$$\therefore \frac{c}{a} = 1.633$$

(b) Show packing Coeff = 0.74

$12 \times \frac{1}{6}$th atoms + 3 whole atoms + $2 \times \frac{1}{2}$ atoms

= 6 atoms / cell

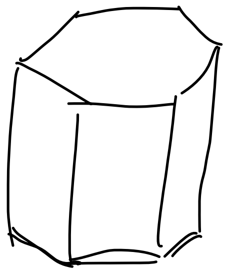
Close packed on bottom edges

$2r = a$

also $\frac{c}{a} = \sqrt{8/3} \rightarrow c = \sqrt{\frac{8}{3}}\, a = 2\sqrt{\frac{8}{3}}\, r$

Volume atoms $= 6 \times \frac{4}{3}\pi r^3$

base area



c

Volume cell $= c \cdot \left[\frac{3\sqrt{3}}{2} a^2\right]$

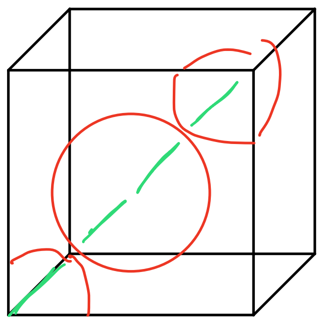
$= \left[2\sqrt{\frac{8}{3}}\, r\right]\left[\frac{3\sqrt{3}}{2}(2r)^2\right]$

$$\frac{8\pi r^3}{\left[2\sqrt{\frac{8}{3}}\, r\right]\left[\frac{3\sqrt{3}}{2}(2r)^2\right]} = \frac{\pi}{\sqrt{\frac{8}{3}} \times \frac{3\sqrt{3}}{2}}$$

$$= \frac{\pi}{3\sqrt{2}}$$

$$\approx 0.74048$$

now for FCC



for FCC

4 atoms/cell $\rightarrow 4\left[\frac{4}{3}\pi r^3\right]$

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

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

$$V = a^3 = \left[\frac{4}{\sqrt{2}} r\right]^3 = \frac{64}{2\sqrt{2}} r^3$$

$$APF = \frac{\frac{16}{3}\pi r^3}{\frac{64}{2\sqrt{2}} r^3} = \frac{16}{3} \times \frac{2\sqrt{3}}{64}\pi$$

$$= \frac{2\sqrt{2}}{12}\pi$$

$$= \frac{\sqrt{3}}{6}\pi$$

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

$$= \frac{1}{3\sqrt{2}}\pi$$