CTM - Gabarito - Exercícios - 2016.1

I Unidade

① -

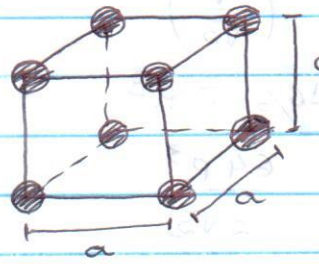
$$\text{Nº átomos} = \frac{\text{massa (g)} \times N_A \text{ (átomos/mol)}}{A \text{ (g/mol)}}$$

$$\text{Nº átomos} = \frac{100\,(g) \times 6{,}023 \times 10^{23}\ (\text{átomos/mol})}{107{,}87\ (g/mol)}$$

$$\boxed{\text{Nº átomos} = 5{,}58 \times 10^{23} \text{ átomos}}$$

② -

(a) Metal CS ; a = ? e FEA = ?



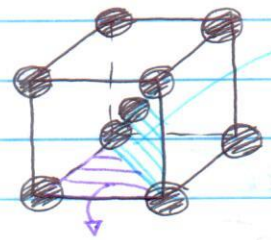
$$\boxed{a = 2R}$$

$$\text{FEA} = \frac{\text{volume átomos}}{\text{volume célula unitária}}$$

$$\text{FEA} = \frac{1 \cdot 4/3\ \pi R^3}{a^3} = \frac{4/3\ \pi R^3}{(2R)^3} = \frac{4/3\ \pi R^3}{8R^3} = \frac{4}{3}\pi \cdot \frac{1}{8}$$

$$\boxed{\text{FEA} = \frac{\pi}{6} = 0{,}52 \text{ ou } 52\%}$$

(b) Metal CCC ; a = ? e FEA = ?



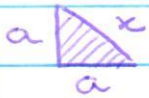
$$(4R)^2 = a^2 + (a\sqrt{2})^2$$

$$16R^2 = a^2 + 2a^2$$

$$3a^2 = 16R^2$$

$$a^2 = \frac{16R^2}{3}$$

$$a = \sqrt{\frac{16R^2}{3}}$$



$$x^2 = a^2 + a^2$$

$$x = \sqrt{2a^2}$$

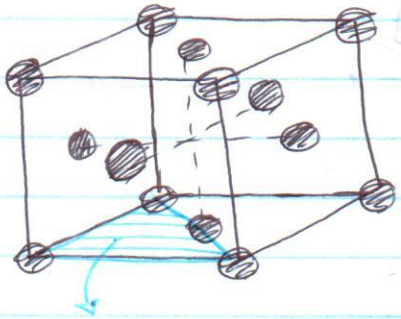
$$x = a\sqrt{2}$$

$$\boxed{a = \frac{4R}{\sqrt{3}}}$$

$$FEA = \frac{2 \cdot 4/3 \cdot \pi R^3}{a^3} = \frac{8/3\ \pi R^3}{\left(\frac{4R}{\sqrt{3}}\right)^3} = \frac{8/3\ \pi R^3}{\frac{64 R^3}{3\sqrt{3}}} =$$

$$FEA = \frac{8}{3}\pi R^3 \times \frac{3\sqrt{3}}{64 R^3} = \frac{\pi\sqrt{3}}{8} = \underline{0{,}68 \text{ ou } 68\%} \quad //$$

(c) Metal CFC ; a = ? e FEA = ?

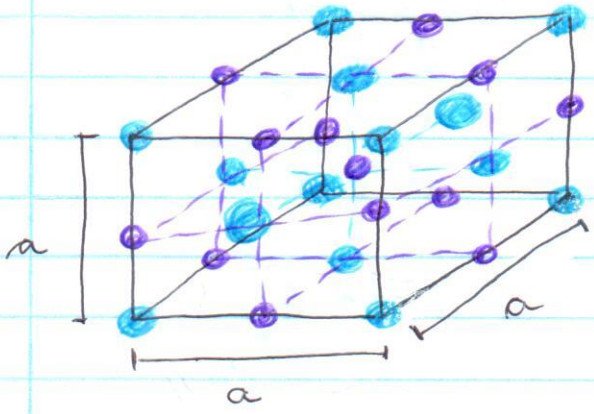


$$(4R)^2 = a^2 + a^2$$
$$16R^2 = 2a^2$$
$$a^2 = \frac{16R^2}{2}$$
$$a = \sqrt{\frac{16R^2}{2}}$$

$$\boxed{a = \frac{4R}{\sqrt{2}}} \quad //$$

$$FEA = \frac{4 \cdot 4/3\ \pi R^3}{a^3}$$
$$= \frac{(16/3)\pi R^3}{\left(\frac{4R}{\sqrt{2}}\right)^3}$$
$$= \frac{16/3\ \pi R^3}{\frac{64 R^3}{2\sqrt{2}}}$$
$$= \frac{16}{3}\pi R^3 \times \frac{2\sqrt{2}}{64 R^3}$$
$$= \frac{\pi\sqrt{2}}{6} = \underline{0{,}74 \text{ ou } 74\%} \quad //$$

(d) NaCl ; a = ? e FEI = ?



● Cl^-
● Na^+

$$\boxed{a = 2R_{Cl^-} + 2R_{Na^+}} \quad //$$

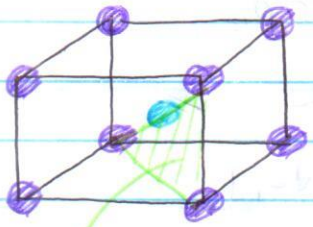
$$FEI = \frac{n_{e^-} V_{e^-} + n_{Na^+} V_{Na^+}}{a^3}$$

$$= \frac{\left[4 \cdot 4/3 \cdot \pi \cdot R_{e^-}^3\right] + \left[4 \cdot 4/3 \cdot \pi \cdot R_{Na^+}^3\right]}{\left[2 R_{e^-} + 2 R_{Na^+}\right]^3}$$

$$= \frac{\left[16/3 \cdot \pi \cdot 0,181^3\right] + \left[16/3 \cdot \pi \cdot 0,102^3\right]}{\left[2 \cdot 0,181 + 2 \cdot 0,102\right]^3}$$

$$= \frac{0,0993 + 0,0178}{0,1813} = 0,64 \text{ ou } 64\%$$

(e) e_{sel} ; $a = ?$ e $FEI = ?$



e^-

e_s^+

$$(2R_{cl} + 2R_{es})^2 = (a\sqrt{2})^2 + a^2$$

$$2a^2 + a^2 = (2R_{cl} + 2R_{es})^2$$

$$a^2 = \frac{(2R_{cl} + 2R_{es})^2}{3}$$

$$a = \frac{2R_{cl} + 2R_{es}}{\sqrt{3}}$$

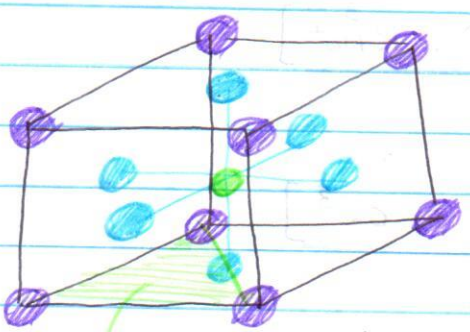
$$FEI = \frac{\left[1 \cdot 4/3\,\pi \cdot R_{cl}^3\right] + \left[1 \cdot 4/3\,\pi \cdot R_{es}\right]}{\left(\frac{2R_{cl} + 2R_{es}}{\sqrt{3}}\right)^3}$$

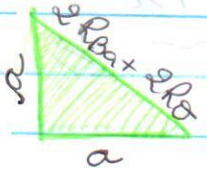
$$FEI = \frac{\left[4/3\,\pi \cdot 0,181^3\right]}{\left(\frac{2 \cdot 0,181 + 2 \cdot 0,170}{\sqrt{3}}\right)^3} + \frac{\left[4/3\,\pi \cdot 0,170^3\right]}{\left(\frac{2 \cdot 0,181 + 2 \cdot 0,170}{\sqrt{3}}\right)^3} = 0,68 \text{ ou } 68\%$$

$\equiv 0,025$ $\equiv 0,020$

$= 0,0665$

f) $BaTiO_3$; a = ? e FEI = ?





$$(2R_{Ba} + 2R_O)^2 = a^2 + a^2$$

$$2a^2 = (2R_{Ba} + 2R_O)^2$$

$$a = \sqrt{\frac{(2R_{Ba} + 2R_O)^2}{2}}$$

$$\boxed{a = \frac{2R_{Ba} + 2R_O}{\sqrt{2}}}$$

$$FEI = \frac{[n_{Ba} \cdot V_{Ba}] + [n_O \cdot V_O] + [n_{Ti} \cdot V_{Ti}]}{a^3}$$

$$= \frac{[1 \cdot 4/3 \cdot \pi \cdot 0{,}136^3] + [3 \cdot 4/3 \cdot \pi \cdot 0{,}140^3] + [1 \cdot 4/3 \cdot \pi \cdot 0{,}068^3]}{\left[\frac{2 \cdot 0{,}136 + 2 \cdot 0{,}140}{\sqrt{2}}\right]^3}$$

$$= \frac{0{,}0105 + 0{,}03448 + 1{,}317 \times 10^{-3}}{0{,}0593} = \frac{0{,}0463}{0{,}0593}$$

$$\boxed{FEI = 0{,}78 \text{ ou } 78\%}$$

(3)

a) Alumínio CFC; $R_{Al} = 0,143$ nm, $A_{Al} = 26,98$ g/mol

→ $n = 4$ e $a = 4R/\sqrt{2}$

$$\rho = \frac{n A}{V_C N_A} = \frac{4 \cdot 26,98}{\left(\frac{4 \cdot 0,143 \times 10^{-7}}{\sqrt{2}}\right)^3 \times 6,023 \times 10^{23}}$$

$$\rho = \frac{107,92}{6,62 \times 10^{-23} \cdot 6,023 \times 10^{23}} \rightarrow \rho = 2,7 \text{ g/cm}^3$$

b) NaCl → $n_{Na} = 4$, $n_{Cl} = 4$ → $a = 2R_{Cl} + 2R_{Na}$

$R_{Cl} = 0,181$ nm
$A_{Cl} = 35,45$ g/mol
$R_{Na} = 0,102$ nm
$A_{Na} = 22,99$ g/mol

$$\rho = \frac{n_{Na} A_{Na} + n_{Cl} A_{Cl}}{(2R_{Cl} + 2R_{Na})^3 \cdot 6,023 \times 10^{23}}$$

$$\rho = \frac{4 \cdot 22,99 + 4 \cdot 35,45}{\left[2^3 \cdot (10^{-7})^3 \cdot (0,181 + 0,102)^3\right] \cdot 6,023 \times 10^{23}} =$$

$$\rho = \frac{233,76}{[18,13 \times 10^{-23}] \cdot [6,023 \times 10^{23}]} \rightarrow \rho = 2,1 \text{ g/cm}^3$$

c) Ferro CCC; $R_{Fe} = 0,124$ nm e $A_{Fe} = 55,85$ g/mol

→ $n = 2$ e $a = 4R/\sqrt{3}$

$$\rho = \frac{2 \cdot 55,85}{\left[\frac{4 \cdot 0,124 \times 10^{-7}}{\sqrt{3}}\right]^3 \cdot 6,023 \times 10^{23}} = \frac{111,7}{2,35 \times 10^{-23} \cdot 6,023 \times 10^{23}}$$

$$\rho = 7,9 \text{ g/cm}^3$$

d) CsCl → $n_{Cs} = 1$
$n_{Cl} = 1$
$a = \frac{2R_{Cs} + 2R_{Cl}}{\sqrt{3}}$

$R_{Cs} = 0,170$ nm
$A_{Cs} = 132,9$ g/mol
$R_{Cl} = 0,181$ nm
$A_{Cl} = 35,45$ g/mol

$$\rho = \frac{1 \cdot 132,9 + 1 \cdot 35,45}{\left[\frac{2 \cdot 0,170 \times 10^{-7} + 2 \cdot 0,181 \times 10^{-7}}{\sqrt{3}}\right]^3 \cdot 6,023 \times 10^{23}}$$

$$\rho = \frac{168,35}{6,66 \times 10^{-23} \cdot 6,023 \times 10^{23}} \rightarrow \boxed{\rho = 4,2 \text{ g/cm}^3}$$

e) Titânio HC ; $R_{Ti} = 0,145$ nm
$A_{Ti} = 47,87$ g/mol
$n = 6$
$a = 2R$
$c = \frac{\sqrt{8}}{\sqrt{3}} a$
$V_c = 24 R^3 \sqrt{2}$

$$\rho = \frac{6 \cdot 47,87}{\left[24 \cdot (0,145 \times 10^{-7})^3 \cdot \sqrt{2}\right] \cdot 6,023 \times 10^{23}}$$

$$\rho = \frac{287,22}{10,35 \times 10^{-23} \cdot 6,02 \times 10^{23}} \rightarrow \boxed{\rho = 4,6 \text{ g/cm}^3}$$

f) $BaTiO_3$; $R_{Ba} = 0,136$ nm ; $A_{Ba} = 137,32$ g/mol
$R_{Ti} = 0,068$ nm ; $A_{Ti} = 47,87$ g/mol
$R_O = 0,140$ nm ; $A_O = 16$ g/mol

$n_{Ba} = 1$
$n_{Ti} = 1$
$n_O = 3$
$a = \frac{2R_{Ba} + 2R_O}{\sqrt{2}}$

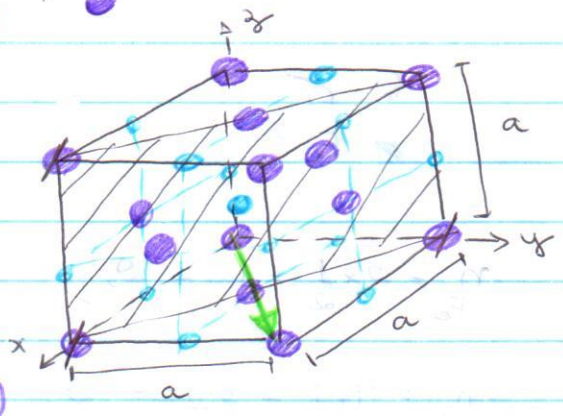
$$\rho = \frac{[1 \cdot 137,32] + [1 \cdot 47,87] + [3 \cdot 16]}{\left[\frac{2 \cdot 0,136 \times 10^{-7} + 2 \cdot 0,140 \times 10^{-7}}{\sqrt{2}}\right]^3 \cdot 6,023 \times 10^{23}}$$

$$\rho = \frac{233,19}{5,95 \times 10^{-23} \cdot 6,023 \times 10^{23}} \rightarrow \boxed{\rho = 6,5 \ g/cm^3}$$

④

$FeO \rightarrow AX \rightarrow$ NC = 6 → semelhante ao Na^+Cl^-
NC = 8 → semelhante ao Cs^+Cl^-
NC = 4 → semelhante ao Zn^+S^-

Fe^+ ; O^-



$n_{Fe} = 4$
$n_O = 4$

[1 1 0]
(1 1 0)

ⓐ
$a = 2R_{Fe} + 2R_O = 2 \cdot 0,140 + 2 \cdot 0,133 = 0,546 \ nm$

ⓑ $FEI = \frac{n_{Fe} V_{Fe} + n_O V_O}{a^3} = \frac{\left[4 \cdot \frac{4}{3} \pi \cdot 0,133^3\right] + \left[4 \cdot \frac{4}{3} \pi \cdot 0,140^3\right]}{(0,546)^3}$

$FEI = \frac{0,039 + 0,046}{0,163} = 0,52$ ou 52%

ⓒ
$\rho = \frac{n_{Fe} A_{Fe} + n_O A_O}{V_c \cdot N_A} = \frac{4 \cdot 55,85 + 4 \cdot 16}{(0,546 \times 10^{-7})^3 \cdot (6,023 \times 10^{23})}$

$\rho = \frac{287,4}{98,04} \rightarrow \boxed{\rho = 2,9 \ g/cm^3}$

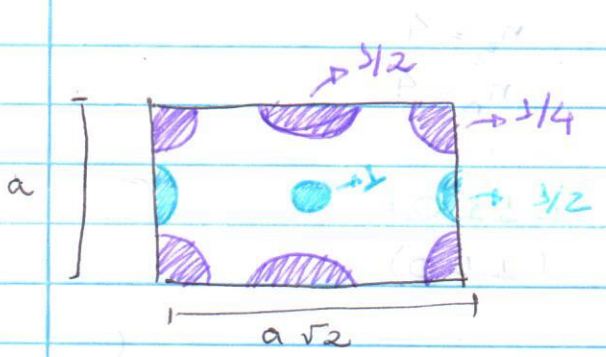
d) DIL → [1 1 0]

$$DIL = \frac{n^{\circ}\ \text{de íons}}{\text{comprimento da direção}}$$

$$DIL = \frac{2\ ce^-}{a\sqrt{2}} = \frac{2\ ce^-}{0,546.\sqrt{2}\ nm} = \frac{2\ ce^-}{0,77}$$

$$DIL \cong 2,6\ ce^- / nm$$

e) DIP → (1 1 0)



$$n_{Fe} = 2 \times \frac{1}{2} + 1 = 2$$

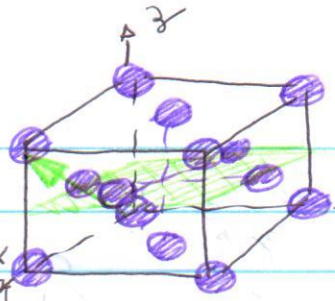
$$n_{O} = 4 \times \frac{1}{4} + 2 \cdot \frac{1}{2} = 2$$

$$DIP = \frac{n^{\circ}\ \text{íons}}{\text{área do plano}} = \frac{2\ O^- + 2\ Fe^+}{a \cdot a\sqrt{2}}$$

$$DIP = \frac{2\ O^- + 2\ Fe^+}{0,546^2.\sqrt{2}} = \frac{2\ (O^- + Fe^+)}{0,421}$$

$$DIP \cong 9,5\ (O^- + Fe^+) / nm^2$$

⑤ Au → cFe



(002)

n = 4

a)

$$a = \frac{4R}{\sqrt{2}} = \frac{4 \cdot 0{,}144}{\sqrt{2}} = 0{,}407 \text{ nm}$$

[101]

b)

$$FEA = \frac{\text{vol. átomos}}{\text{vol. cel. unit.}} = \frac{4 \cdot \frac{4}{3}\pi \cdot R^3}{\left(\frac{4R}{\sqrt{2}}\right)^3} = \frac{\frac{16}{3}\pi R^3}{\frac{64R^3}{2\sqrt{2}}} =$$

$$= \frac{16}{3}\pi R^3 \times \frac{2\sqrt{2}}{64R^3} = \frac{32\pi\sqrt{2}}{3 \cdot 64} = \frac{\pi\sqrt{2}}{6} = 0{,}74 \text{ ou } 74\%$$

c)

$$\rho = \frac{n \cdot A}{Vc \cdot N_A} = \frac{4 \cdot 197}{(0{,}407 \times 10^{-7})^3 \cdot 6{,}023 \times 10^{23}}$$

$$\rho = \frac{788}{40{,}6} \rightarrow \boxed{\rho = 19{,}4 \text{ g/cm}^3}$$

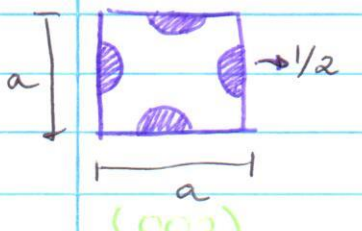
d) DAL → [101]

[101]

$$DAL = \frac{\text{comprimento de átomos}}{\text{comprimento da direção}} = \frac{4R}{a\sqrt{2}}$$

$$= \frac{4R}{\frac{4R}{\sqrt{2}} \cdot \sqrt{2}} = 1 \text{ ou } 100\%$$

e) DAP → (002) → $(0^x, 0^y, 1/2^z)$



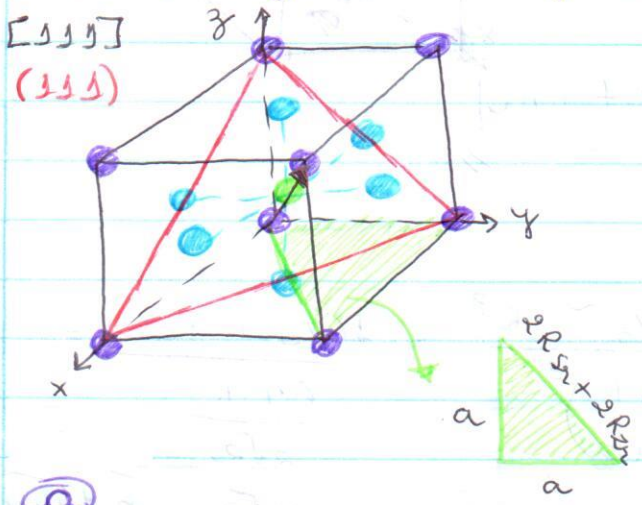
$$DAP = \frac{\text{área de átomos}}{\text{área do plano}} = \frac{2 \cdot \pi R^2}{a^2} =$$

$$= \frac{2\pi R^2}{\left(\frac{4R}{\sqrt{2}}\right)^2} = \frac{2\pi R^2}{\frac{16R^2}{2}} = 2\pi R^2 \times \frac{\sqrt{2}}{16R^2} = \frac{\pi\sqrt{2}}{8} = 0{,}55 \text{ ou } 55\%$$

⑥

$SrZrO_3 \rightarrow A_mB_nX_p \rightarrow m = n$

↳ semelhante ao $BaTiO_3$



$Sr^{+} \rightarrow \bullet \rightarrow 8 \times \frac{1}{8} = 1$

$O^{-} \rightarrow \bullet \rightarrow 6 \times \frac{1}{2} = 3$

$Zr^{+} \rightarrow \bullet \rightarrow 1$

ⓐ

$(2R_{Sr} + 2R_O)^2 = a^2 + a^2 \rightarrow 2a^2 = (2R_{Sr} + 2R_O) \rightarrow$

$\rightarrow a = \sqrt{\frac{2R_{Sr} + 2R_O}{\sqrt{2}}} \rightarrow a = \frac{2R_{Sr} + 2R_O}{\sqrt{2}}$

$a = \frac{2 \cdot 0,112 + 2 \cdot 0,140}{\sqrt{2}} \rightarrow a = 0,356 \text{ nm}$

ⓑ

$FEI = \frac{n_{Sr} \cdot V_{Sr} + n_{Zr} \cdot V_{Zr} + n_O \cdot V_O}{a^3} =$

$= \frac{[1 \cdot 4/3\pi \cdot R_{Sr}^3] + [1 \cdot 4/3\pi \cdot R_{Zr}^3] + [3 \cdot 4/3\pi \cdot R_O^3]}{(0,356)^3}$

$= \frac{[4/3\pi \cdot 0,112^3] + [4/3\pi \cdot 0,072^3] + [4\pi \cdot 0,140^3]}{0,0451}$

$= \frac{5,885 \times 10^{-3} + 1,563 \times 10^{-3} + 34,48 \times 10^{-3}}{0,0451} = \frac{0,0419}{0,0451}$

$FEI = 0,93$ ou 93%

ⓒ

$\rho = \frac{n_{Sr} A_{Sr} + n_{Zr} A_{Zr} + n_O A_O}{V_c \cdot N_A}$

$$\rho = \frac{[1 \cdot 87{,}62] + [1 \cdot 91{,}22] + [3 \cdot 16]}{(0{,}356 \times 10^{-7})^3 \cdot (6{,}023 \times 10^{23})} =$$

$$= \frac{226{,}84}{27{,}17} \rightarrow \boxed{\rho = 8{,}3 \text{ g/cm}^3}$$

(d) 

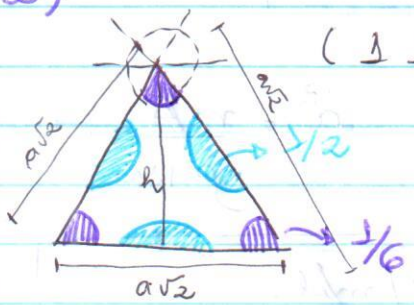
[1 1 1]

$$DIL = \frac{\text{quantidade de íons}}{\text{comprimento da direção}}$$

$$DIL = \frac{1\,Sr^+ + 1\,Zr^+}{a\sqrt{3}} = \frac{1\,(Sr^+ + Zr^+)}{0{,}356 \cdot \sqrt{3}}$$

$$DIL = \frac{1\,(Sr^+ + Zr^+)}{0{,}62} \rightarrow \boxed{DIL \cong 1{,}6\,(Sr^+ + Zr^+) \text{ /nm}}$$

(e)

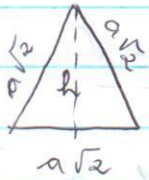


(1 1 1)

$$Sr = 3 \times \frac{1}{6} = 1/2 \text{ átomo}$$

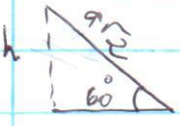
$$O = 3 \times \frac{1}{2} = 3/2 \text{ átomo}$$

OBS! o átomo central (Zr^+) não está contido no plano (111) porque este plano faz um ângulo de 45° em relação ao centro da célula unitária e por isso não passa pelo centro do átomo de Zr^+.



$$\text{Área} = \frac{b \times h}{2} = \frac{a\sqrt{2} \cdot a\sqrt{6}/2}{2} = \frac{a^2\sqrt{12}}{4} \times \frac{2}{1}$$

$$\text{Área} = a^2\sqrt{12}$$



$$\sin 60° = \frac{h}{a\sqrt{2}} \rightarrow h = \frac{a\sqrt{6}}{2}$$

$$\frac{\sqrt{3}}{2} = \frac{h}{a\sqrt{2}}$$

DIP = quantidade de íons no plano / área total do plano

$$DIP = \frac{1/2\ Sr^{+} + 3/2\ O^{-}}{a^2\sqrt{12}} = \frac{1/2\ Sr^{+} + 3/2\ O^{-}}{0{,}356^2\sqrt{12}} =$$

$$= \frac{1/2\ Sr^{+} + 3/2\ O^{-}}{0{,}439} \rightarrow DIP \cong 1{,}14\ Sr^{+} + 3{,}42\ O/nm^2$$

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(7) Potássio → K → CCC → n = 2

$\rho = 0{,}855\ g/cm^3$

$A = 39{,}09\ g/mol$

$a = 4R/\sqrt{3}$

a) a = ?

b) R = ?

$R = \frac{a\sqrt{3}}{4}$

$$\rho = \frac{nA}{V_c \cdot N_A} \rightarrow V_c = \frac{nA}{\rho \cdot N_A} \rightarrow a^3 = \frac{nA}{\rho \cdot N_A} \rightarrow$$

$$\rightarrow a = \sqrt[3]{\frac{n \cdot A}{\rho \cdot N_A}} = \sqrt[3]{\frac{2\ \text{átomos} \cdot 39{,}09\ g/mol}{0{,}855\ g/cm^3 \cdot 6{,}023 \times 10^{23}\ \frac{\text{átomos}}{mol}}}$$

$$\rightarrow a = \sqrt[3]{\frac{78{,}18}{(5{,}1497 \times 10^{23})}} = \sqrt[3]{1{,}518 \times 10^{-22}}$$

$\rightarrow a = 5{,}33 \times 10^{-8}\ cm$

ou

$a = 0{,}533 \times 10^{-7}\ cm$

ou

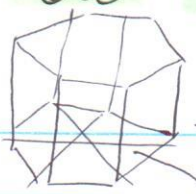
$a = 0{,}533\ nm$

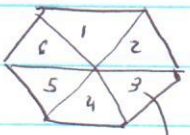
Logo:

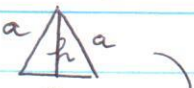
$R = \frac{0{,}533\sqrt{3}}{4}$

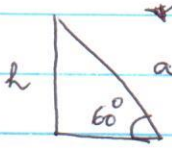
$R = 0{,}231\ nm$

? Qual o volume do HC ?









$\sin 60° = \frac{h}{a}$

$\frac{\sqrt{3}}{2} = \frac{h}{a}$

$h = \frac{\sqrt{3}}{2} a$

$V_c = V_{hexágono}$

$V_c = A_{base} \times altura$

$V_c = 6 . A_{triângulo} \times c$

$V_c = 6 . \frac{b \times h}{2} \times c$

$V_c = 6 . \frac{a \times \frac{\sqrt{3}}{2} a}{2} \times c$

$V_c = 3 . \frac{a^2 \sqrt{3}}{2} . c$

$V_c = \frac{3}{2} . a^2 \sqrt{3} . \frac{\sqrt{8}}{\sqrt{3}} . a$

$V_c = \frac{3\sqrt{8}}{2} a^3$

$V_c = \frac{3 . 2\sqrt{2}}{2} . (2R)^3$

$V_c = 3 . 2^3 . \sqrt{2} . R^3$

$V_c = 3 . 8 . \sqrt{2} . R^3$

$\boxed{V_c = 24 R^3 \sqrt{2}}$

↳ volume da célula unitária hexagonal