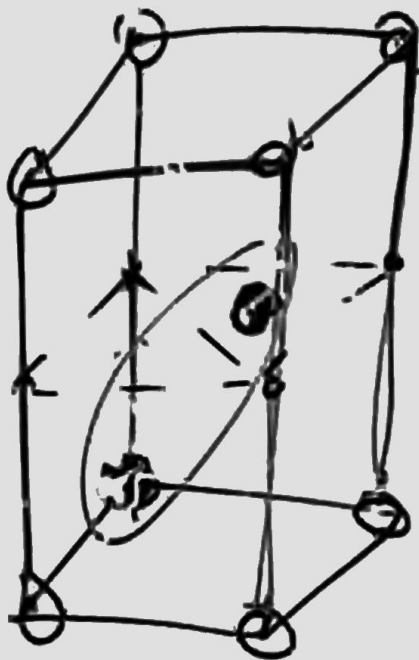


H.C



$$Z = 9 \times \frac{1}{8} + 1 \times 1 = 2$$

2 atoms per unit cell

Sys: hexagonal: mode 2

No. of atoms per unit cell

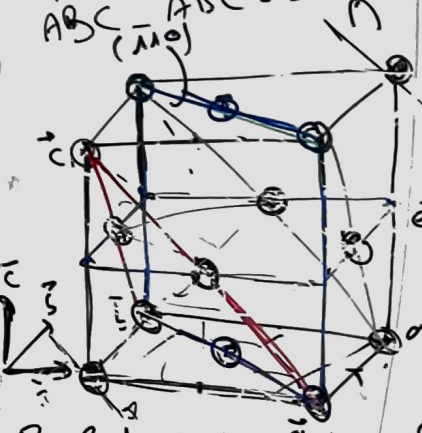
$$\vec{r} = m\vec{a} + n\vec{b} + p\vec{c}$$

1 unit cell contains 2 atoms

$$2 \text{ atoms } (0,0,0); \left(\frac{1}{3}, \frac{2}{3}, \frac{1}{2}\right)$$

I-2: Empilement Capa (1)
 Cubique à faces centrées:
 C.F.C (mode F)

séquence d'empilement:
 ABC (110) ABC ...



$Z = 8 \times \frac{1}{8} + 6 \times \frac{1}{2} = 4$
 $(0,0,0); (\frac{1}{2}, \frac{1}{2}, 0)$
 $(\frac{1}{2}, 0, \frac{1}{2}); (0, \frac{1}{2}, \frac{1}{2})$

A, B, C $\perp$ à la
 face diagonale:
 $d_{A-A} = \frac{a\sqrt{2}}{2}$
 A, B, C: parallèles
 équidistants

$d_{(A,B,C)} \in \hat{m} (hkl)$
 $(A,B,C) \in (111)$

eq distant: $d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$

$d_{hkl} = \frac{a\sqrt{3}}{3} = \frac{a}{\sqrt{3}}$

$d_{hkl} = \frac{a}{\sqrt{1^2 + 1^2 + 1^2}}$

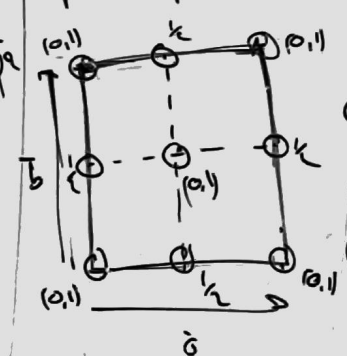
$(hkl): (111)$

Coordonnée N_c

$N_c = 3 + 6 + 3$
 (B) (A) (C)

$N_c = 12$

Projection Capa sur (001)
 passe par l'origine



Capa de atomes: sur
 la petite diagonale: la
 rangée la plus dense:

$d = 2R = \frac{a\sqrt{2}}{2}$
 $4R = a\sqrt{2}$

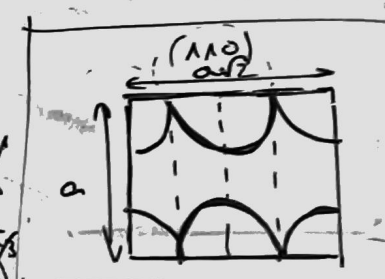
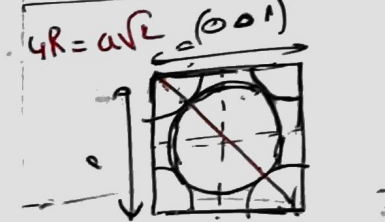
Compacité:

$C = \frac{V_{occ}}{V_{cell}} = \frac{Z \times \frac{4}{3} \pi R^3}{a^3}$

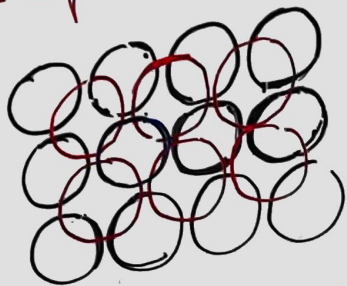
$C = \frac{4 \times \frac{4}{3} \pi R^3}{(2\sqrt{2}R)^3} = \frac{16 \times \frac{4}{3} \pi R^3}{16\sqrt{2}R^3}$

$C = \frac{\pi}{3\sqrt{2}} = 0.74$

Trace de atomes en
 précisant le contact des
 atomes sur:

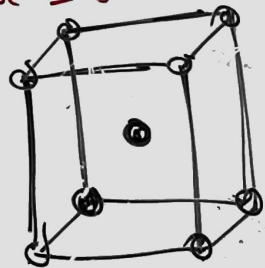


II - Empilement Pseudo Compact : C.C



$\Rightarrow AB - AB \dots \dots \dots$ } C.C

$$N_c = 8$$

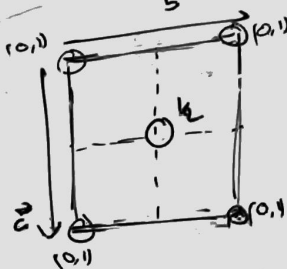


$$Z = 8 \times \frac{1}{8} + 1 \times 1 = 2$$

$$(0,0,0) ; (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$$

$$\rightarrow \frac{(m\vec{a} + n\vec{b} + p\vec{c})}{\vec{a} + \vec{b} + \vec{c}}$$

Projection Cubique de la
maille sur (001)



Calcul de l'atome, angle
diagonale : Rayon le plus
dense

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

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

Compacté : C

$$C = \frac{V_{occ}}{V_{maille}} = \frac{Z \cdot \frac{4}{3} \pi R^3}{a^3}$$

$$C = \frac{2 \times \frac{4}{3} \pi R^3}{(\frac{4R}{\sqrt{3}})^3}$$

$$C = \frac{\frac{8}{3} \pi R^3}{\frac{64 R^3}{3\sqrt{3}}}$$

$$C = \frac{\pi \sqrt{3}}{8} = 0,68 < 0,74$$

la structure n'est pas Compacte

Trace de l'atome en précisant
le contact de l'atome sur :

001



110

$a\sqrt{2}$



$$D = a\sqrt{2} = 4R$$

Empilement Compact: E.C : C.F.C

C.F.C : ABC - ABC

$$N_C = 12 \quad Z = 4$$

$$C = 0,74$$

⇒ 26% de maille: V. de

Empilement Compact: E.C

$$M_b(S.O) = Z$$

$$M_b(S.T) = 2Z$$

C.F.C : Z = 4

$$\begin{cases} M_b(S.O) = 4 \\ M_b(S.T) = 8 \end{cases}$$

R. on du S.T : r_T

$$R + r_T = \frac{a\sqrt{3}}{4} \text{ et } 4R = a\sqrt{2}$$

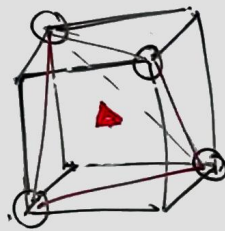
$$R \rightarrow r_T = R\sqrt{\frac{3}{2}}$$

$$r_T = R\left(\sqrt{\frac{3}{2}} - 1\right)$$

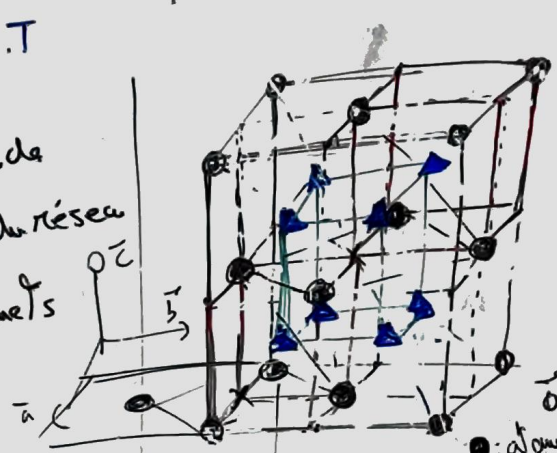
$$r_T = 0,285 R$$

Site tétraédrique : S.T

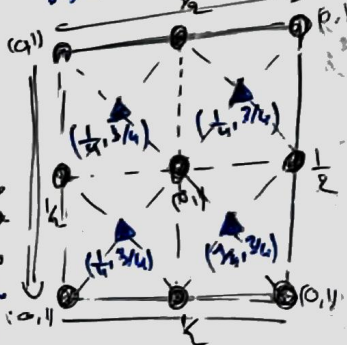
définition : (s) / (u) de
entouré par 4 sphères du réseau
qui occupent les sommets
d'un tétraèdre



le tétraèdre $\begin{cases} 1 \text{ Sommet} \\ 3 \text{ Centres de faces} \\ \text{par le sommet} \end{cases}$



Projection de la
maille et localisation
du centre de S.T. (001)



Position des centres de S.T

• les centres des 8 petits cubes ($\frac{0}{2}$)

• aux $(\frac{1}{4}, \frac{3}{4})$ de chaque g. de
diagonales : 8 S.T par maille

$$(\frac{1}{4}, \frac{1}{4}, \frac{1}{4}) ; (\frac{3}{4}, \frac{1}{4}, \frac{1}{4}) ; (\frac{1}{4}, \frac{3}{4}, \frac{1}{4}) ; (\frac{3}{4}, \frac{3}{4}, \frac{1}{4})$$

$$(\frac{1}{4}, \frac{1}{4}, \frac{3}{4}) ; (\frac{3}{4}, \frac{1}{4}, \frac{3}{4}) ; (\frac{1}{4}, \frac{3}{4}, \frac{3}{4}) ; (\frac{3}{4}, \frac{3}{4}, \frac{3}{4})$$