PRACTICA 4: EMPAQUETAMIENTOS ATOMICOS

Laboratorio de Metalotecnia
ETSIMO

EMPAQUETAMIENOS ATOMICOS

REFERENCIAS BIBLIOGRÁFICAS:

- Capítulo I del libro "CIENCIA E INGENIERIA DE MATERIALES". Prof. José Antonio Pero-Sanz Elorz

Cueva de Naica Chihuahua, México

Cristales de selenita -variedad de yeso hidratado ($CaSO_4.2H_2O$)- de hasta 10 metros de longitud y un metro de ancho.

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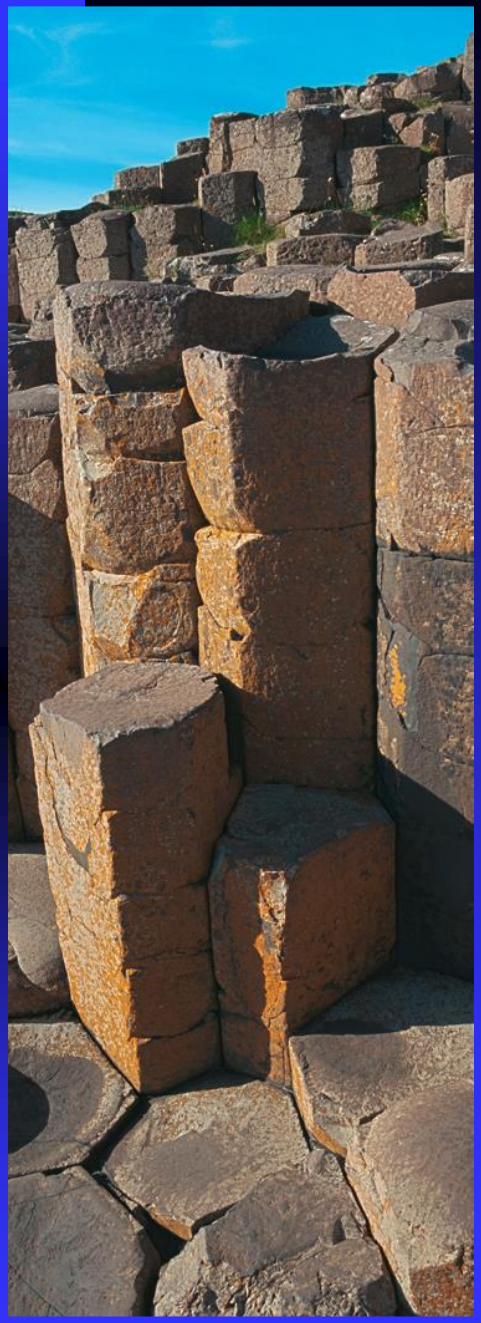
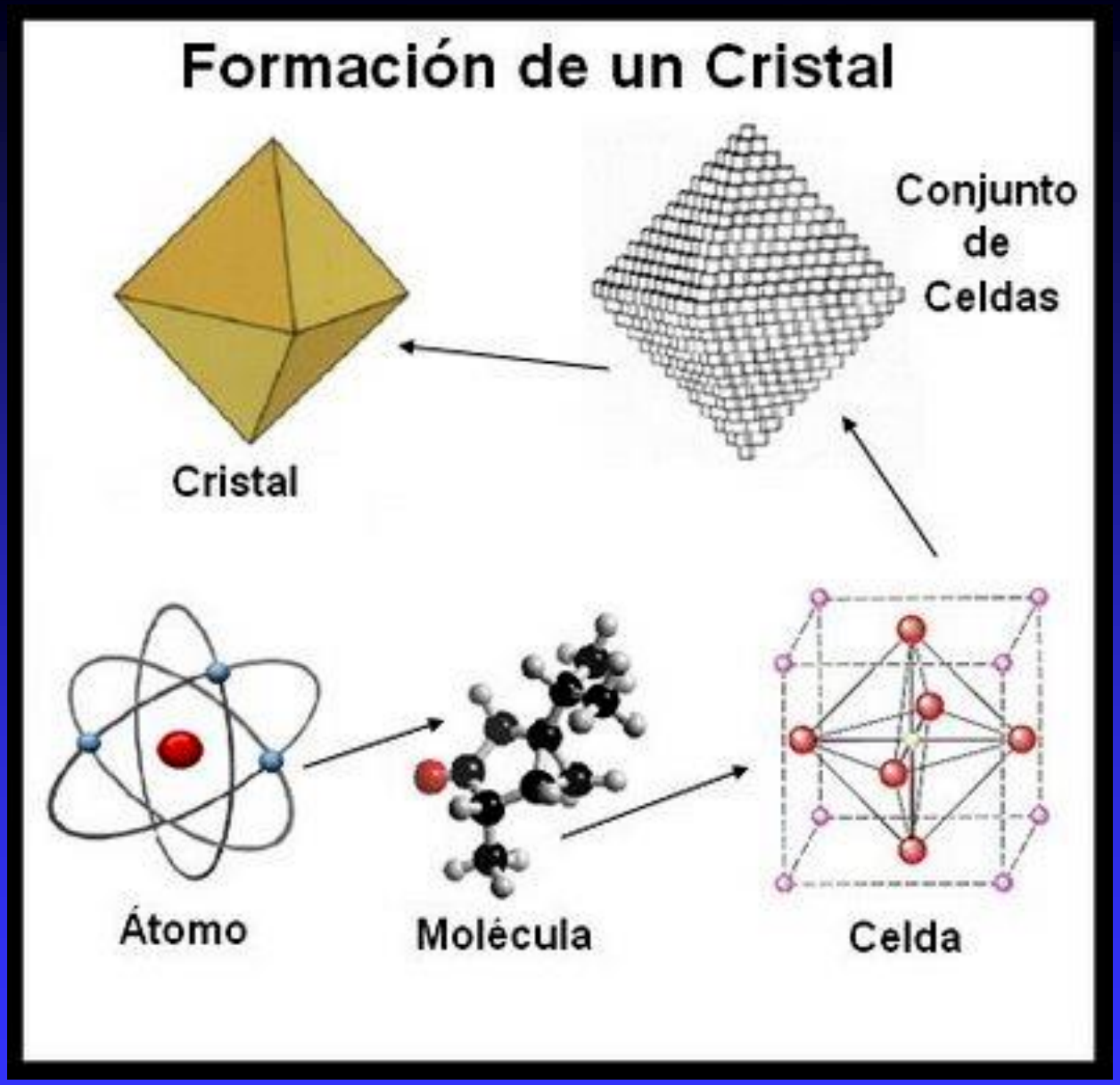
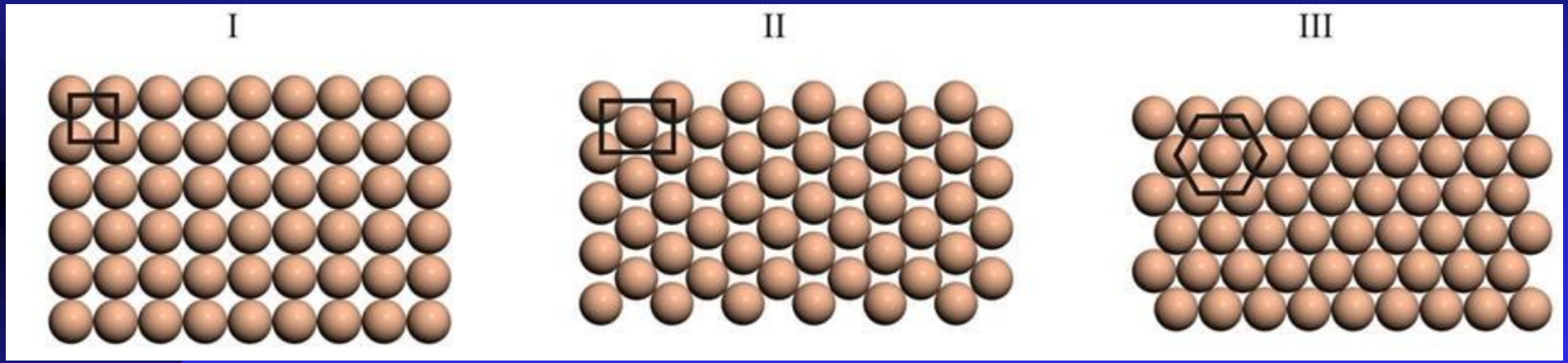


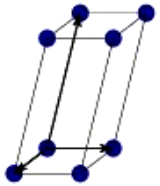
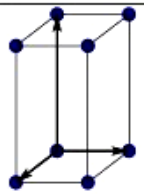
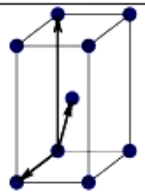
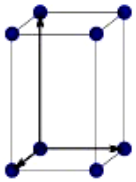
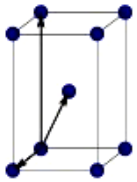
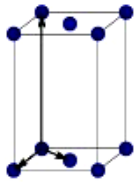
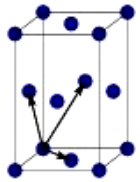
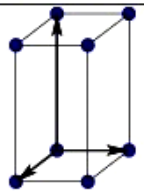
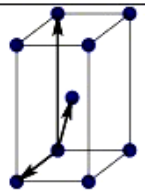
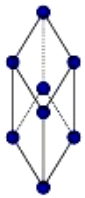
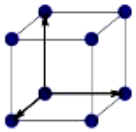
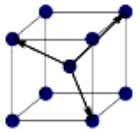
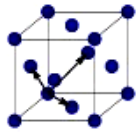
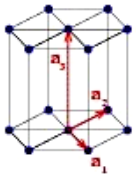
Formación basáltica de la Calzada de los Gigantes, en Irlanda del Norte


Formación de un Cristal
Conjunto de Celdas
Cristal
Átomo
Molécula
Celda

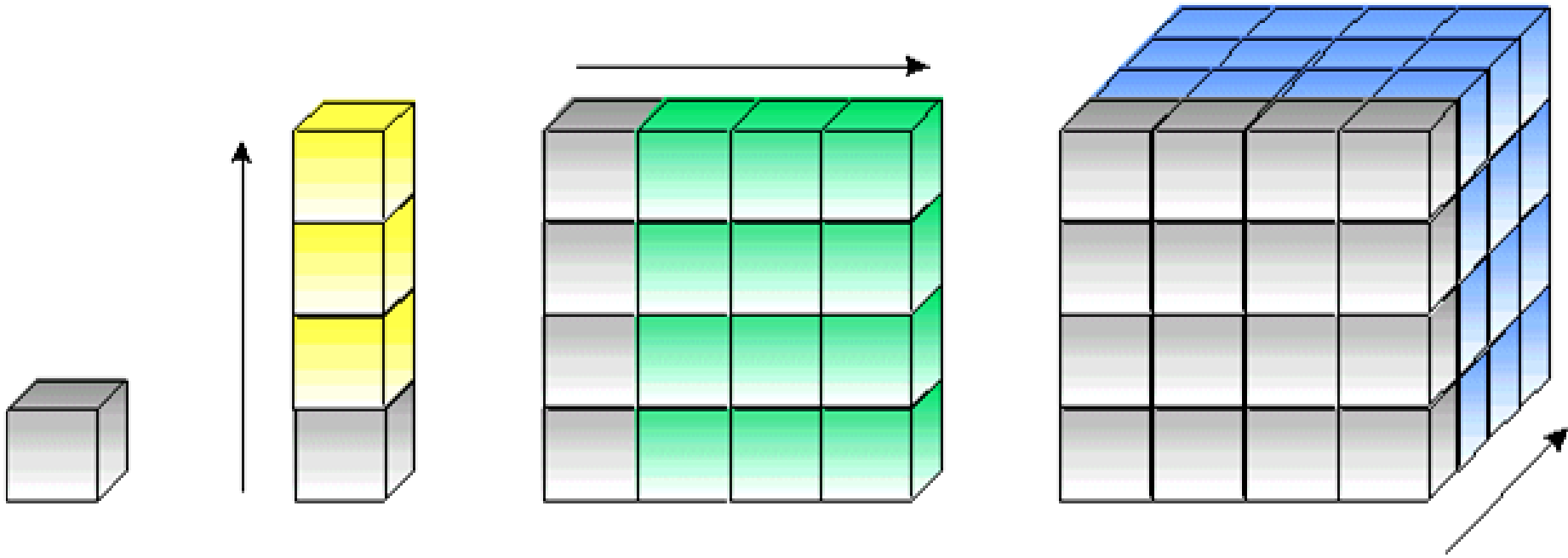
Planos densos



Los planos del tipo III son los mas densos: planos de máxima fracción de empaquetamiento

Bravais lattice	Parameters	Simple (P)	Volume centered (I)	Base centered (C)	Face centered (F)
Triclinic	$a_1 \neq a_2 \neq a_3$ $\alpha_{12} \neq \alpha_{23} \neq \alpha_{31}$				
Monoclinic	$a_1 \neq a_2 \neq a_3$ $\alpha_{23} = \alpha_{31} = 90°$ $\alpha_{12} \neq 90°$				
Orthorhombic	$a_1 \neq a_2 \neq a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} = 90°$				
Tetragonal	$a_1 = a_2 \neq a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} = 90°$				
Trigonal	$a_1 = a_2 = a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} < 120°$				
Cubic	$a_1 = a_2 = a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} = 90°$				
Hexagonal	$a_1 = a_2 \neq a_3$ $\alpha_{12} = 120°$ $\alpha_{23} = \alpha_{31} = 90°$				

SOLIDO CRISTALINO

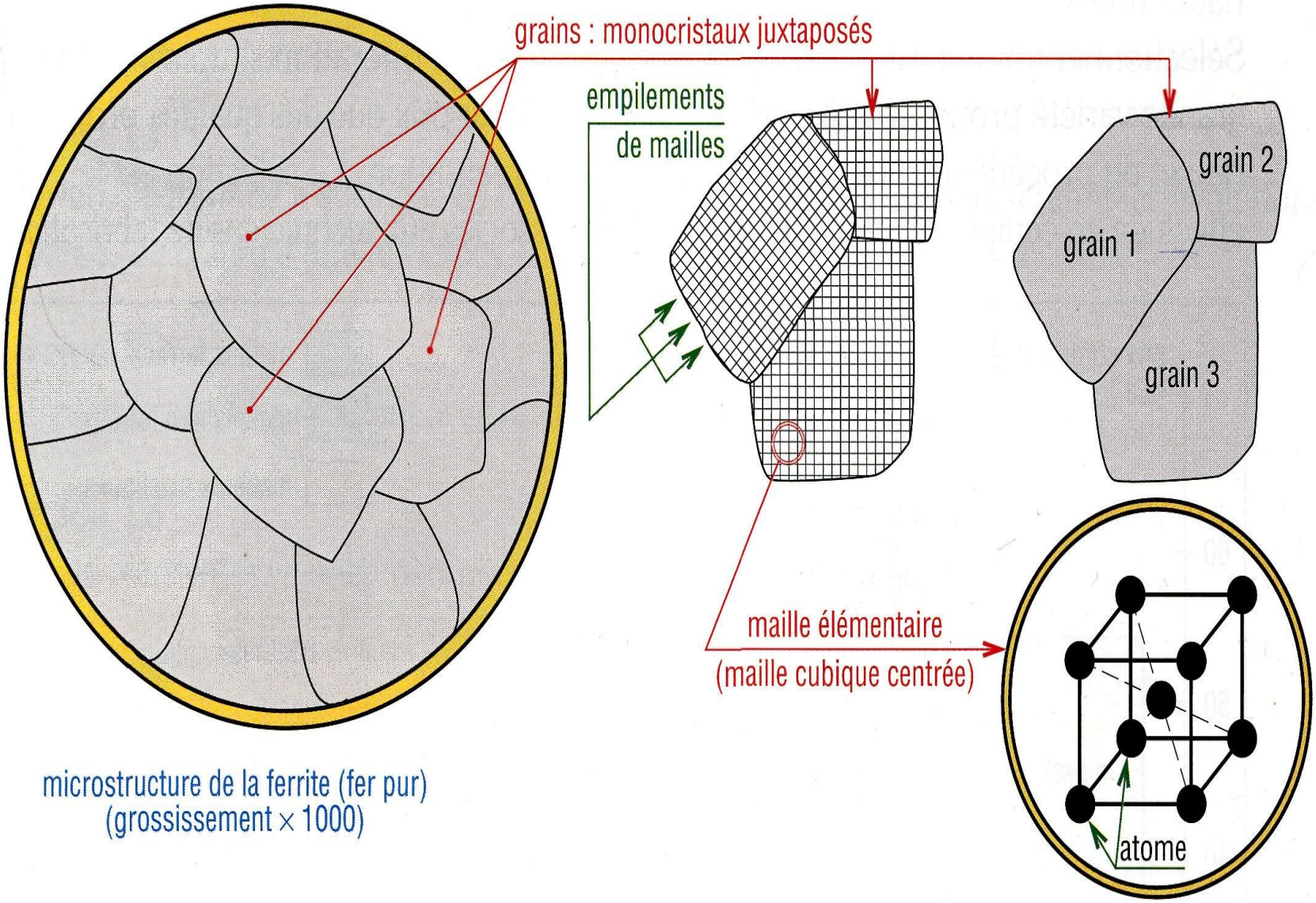


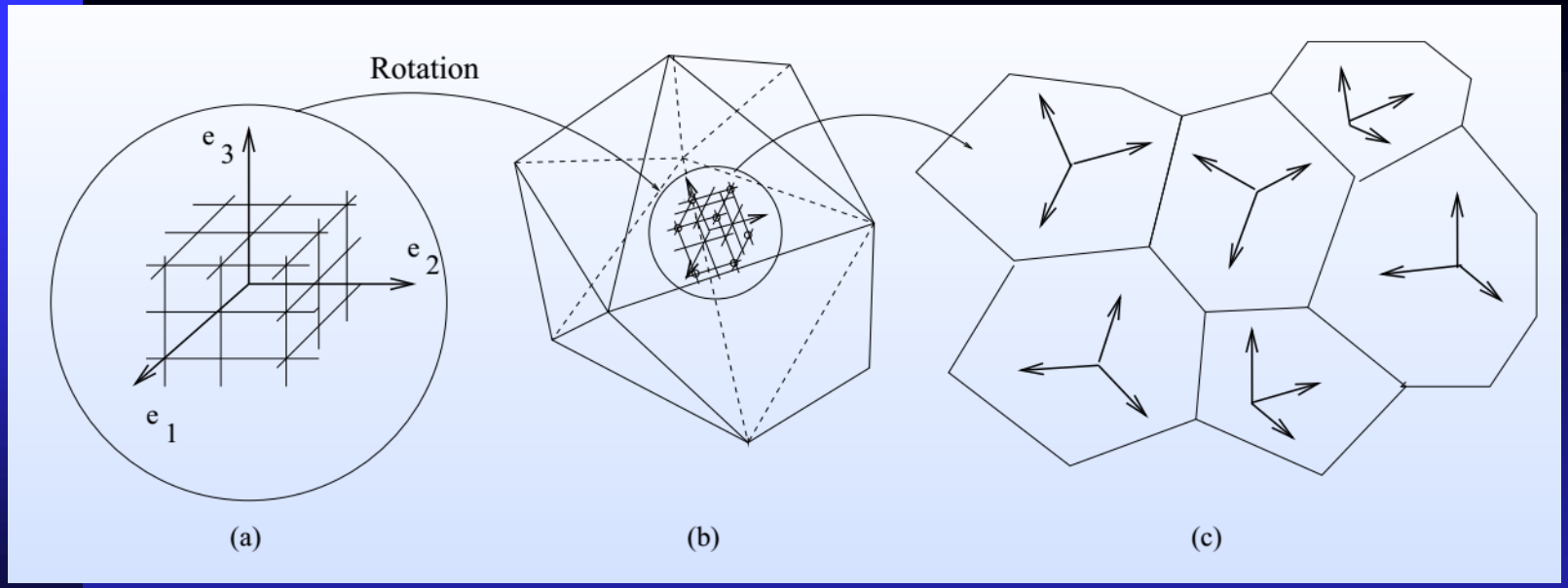
Celda unidad

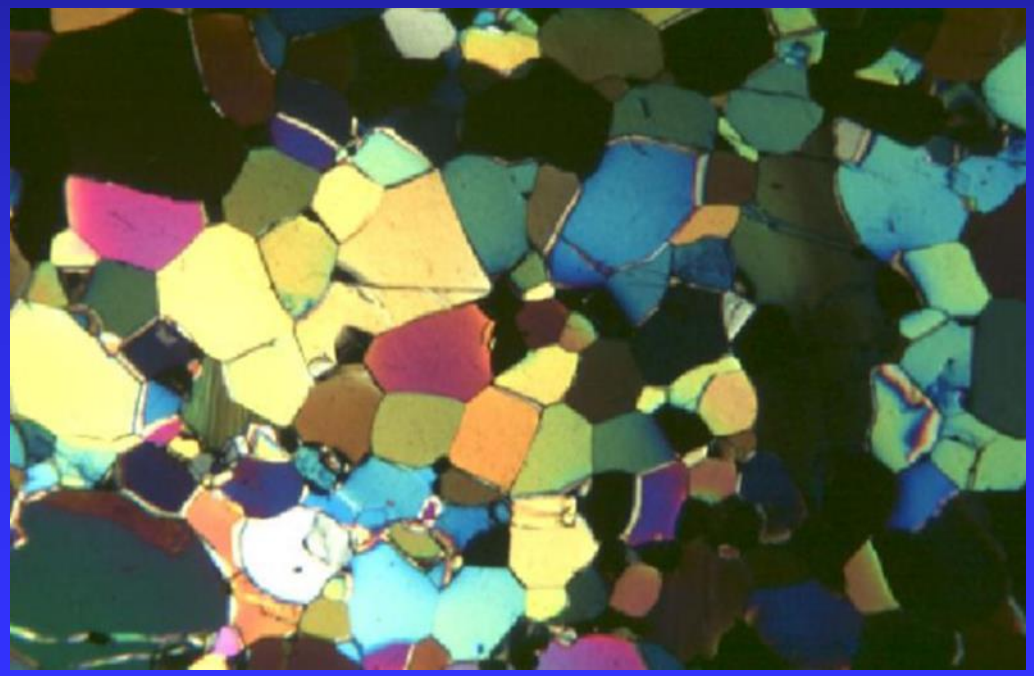
Translación eje Z

Translación eje Y

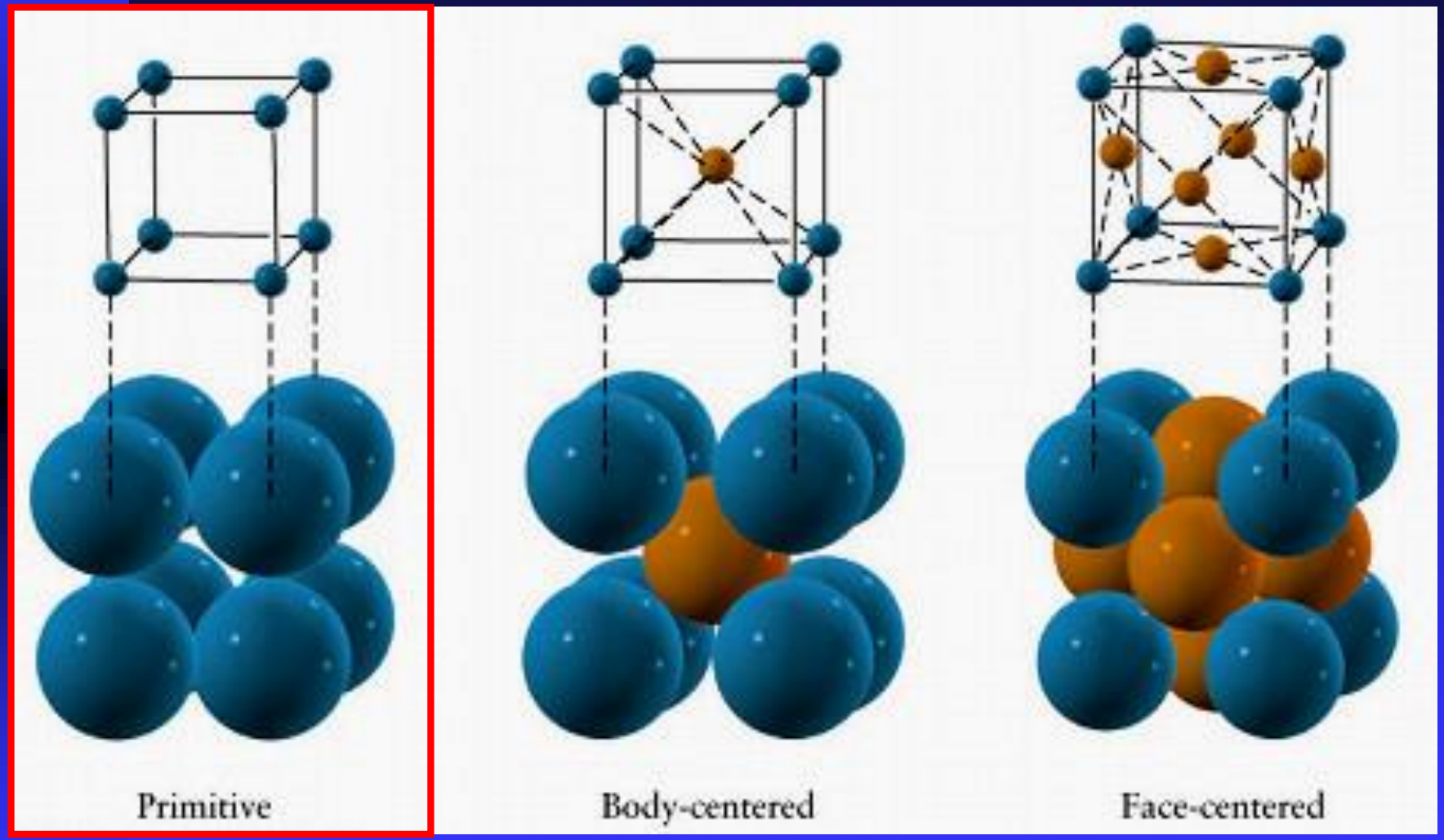
Translación eje X


grains : monocristaux juxtaposés
empilements
de mailles
grain 2
grain 1
grain 3
maille élémentaire
(maille cubique centrée)
atome
microstructure de la ferrite (fer pur)
(grossissement × 1000)

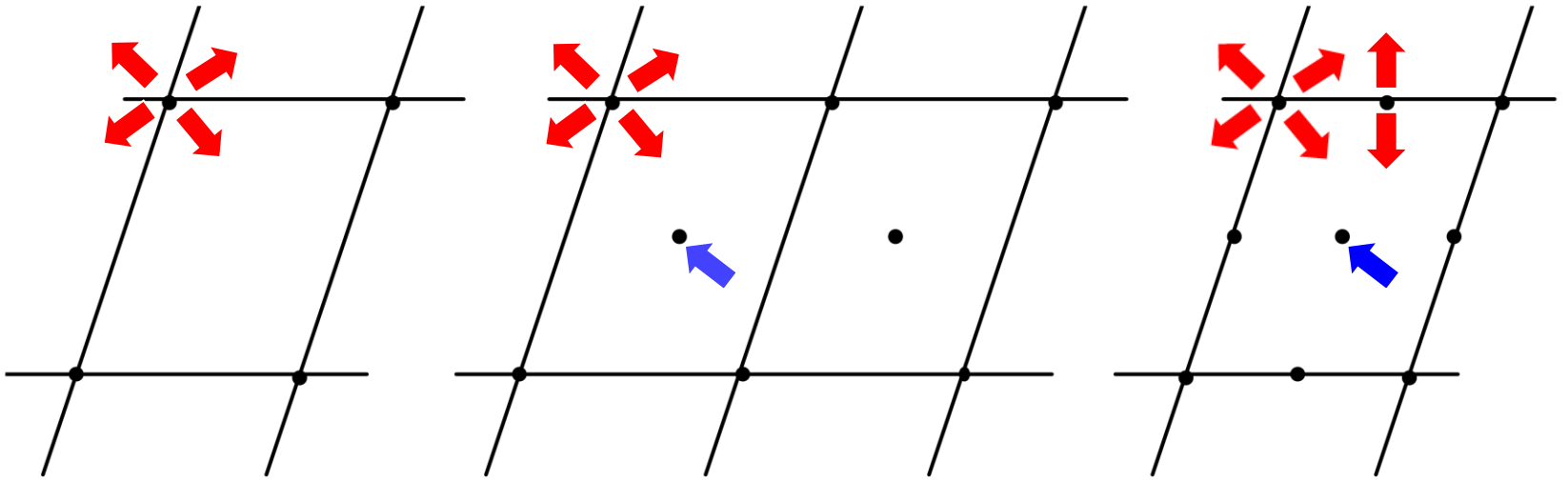

Rotation
e 3
e 2
e 1
(a)
(b)
(c)



RED CUBICA



NUMERO DE ATOMOS PLANARES POR CELDA



(a)

$$n = 4 \times \frac{1}{4} = 1$$

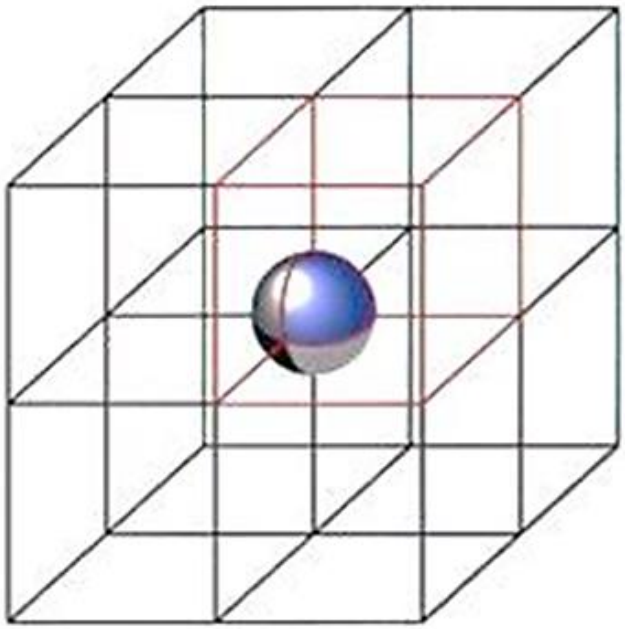
(b)

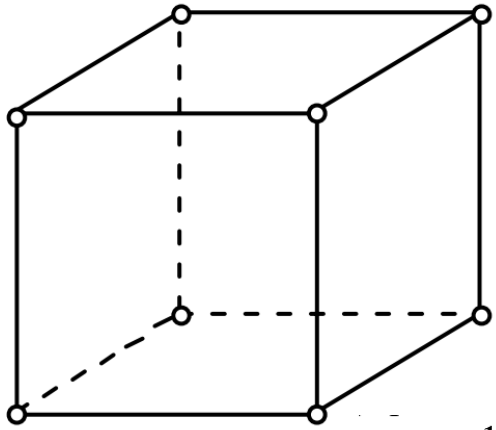
$$n = 4 \times \frac{1}{4} + 1 = 2$$

(c)

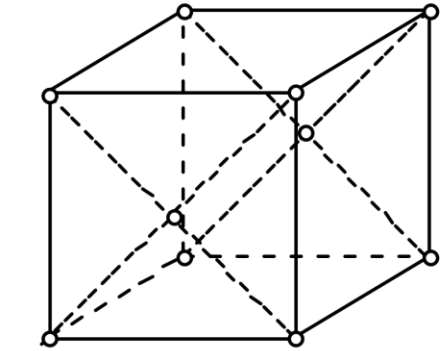
$$4 \times \frac{1}{4} + 4 \times \frac{1}{2} + 1 = 4$$

NUMERO DE ATOMOS POR VOLUMEN EN UNA CELDA



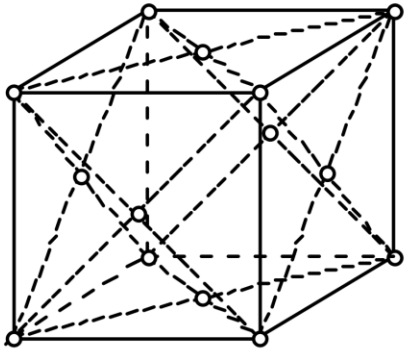


P $m = 8 \times \frac{1}{8} = 1$



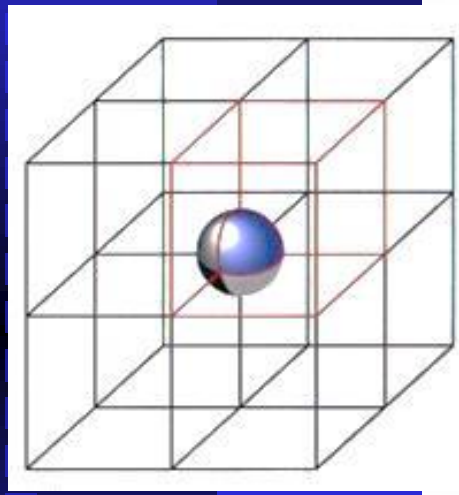
I m = 2

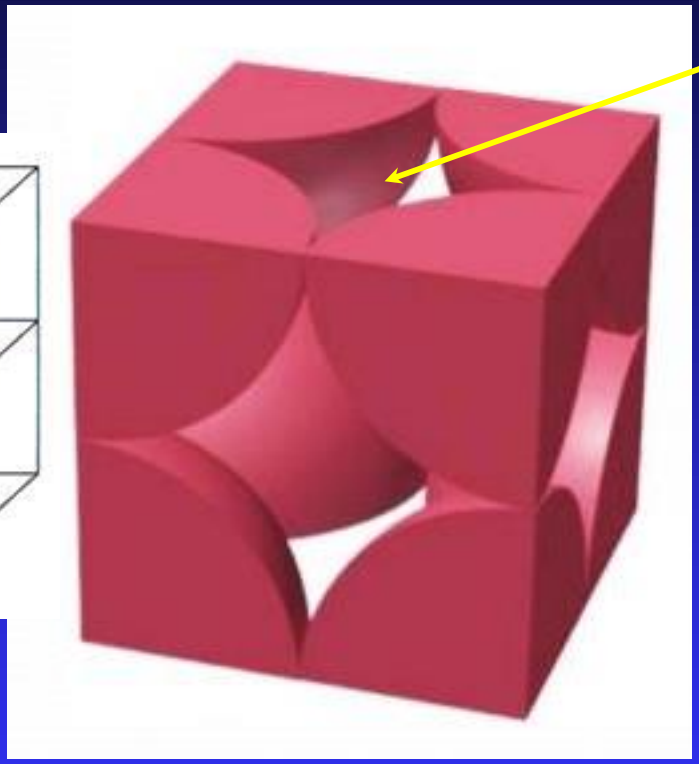
A m = 2



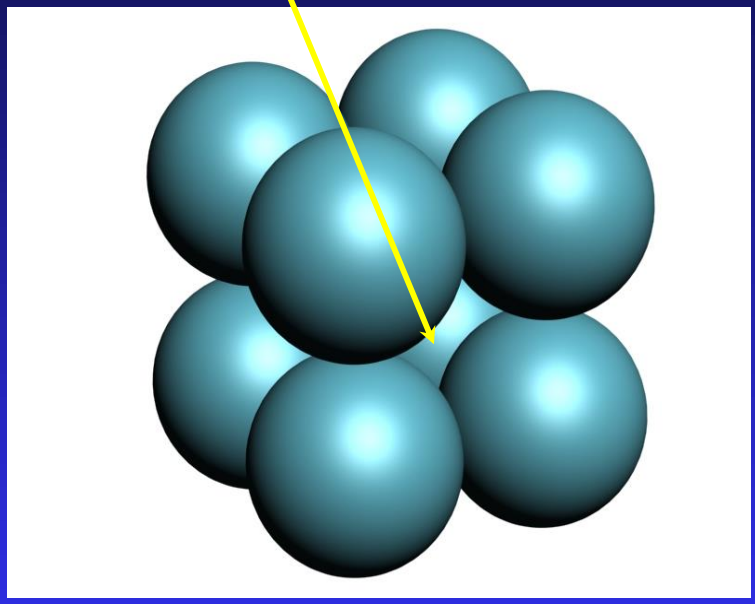
F m = 4

Celda cúbica simple (CS)





Hueco

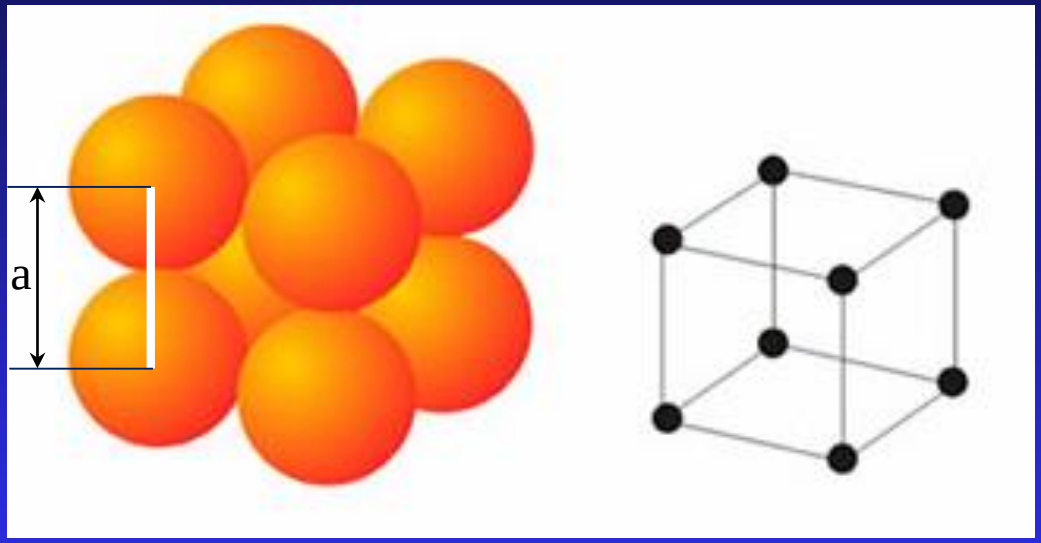


8 vértices . 1/8 = <u>1 átomo</u>

<u>1 átomos / celda</u>

Cristaliza en este sistema: Po

Relación r / a



$$2\,r = a \rightarrow r = \frac{a}{2}$$

Densidad de los materiales

$$\rho_{material} = \frac{M_{atómica}}{V_{celda}} = \frac{n_{átomos} \cdot P_{atómico} / N}{(a_{celda})^3}$$

$P_{a\ metal}$: Tabla I.9, pág. 62

a_{metal} : Tabla I.10, pág. 64

Densidad de materiales CS: Po

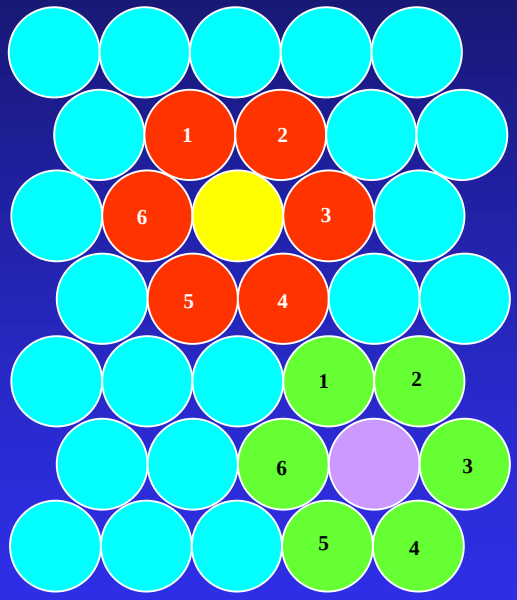
$$\rho_{material} = \frac{M_{atómica}}{V_{celda}} = \frac{n_{átomos} \cdot P_{atómico} / N}{(a_{celda})^3}$$

$$\rho_{Po} = \frac{1\,\text{átomo}\left(\dfrac{210\,\text{g/mol}}{6{,}023.10^{23}\ \text{átomos/mol}}\right)}{\left[3{,}359\,\text{Å}.10^{-8}\ \text{cm/Å}\right]^3} = 9{,}2\,\frac{\text{g}}{\text{cm}^3}$$

$P_{a\ Po}$: 210 g/mol

a_{Po} : 3,359 Å

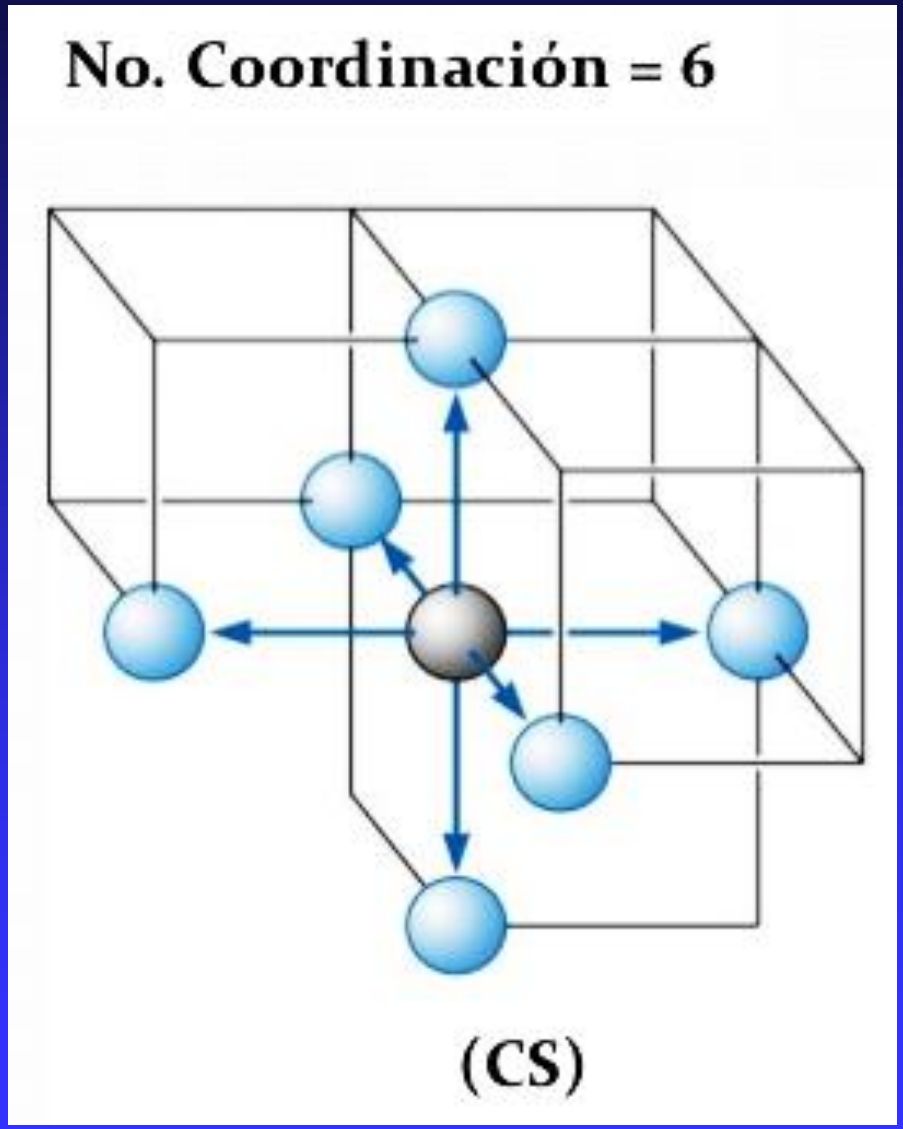
Índice de coordinación



Coordinación 6

Coordination Number	Anion-Cation Radius Ratio	Coordination Geometry
2	> 6.45	
3	4.45–6.45	
4	2.42–4.45	
6	1.37–2.42	
8	1.0–1.37	

Celda cúbica simple (CS)



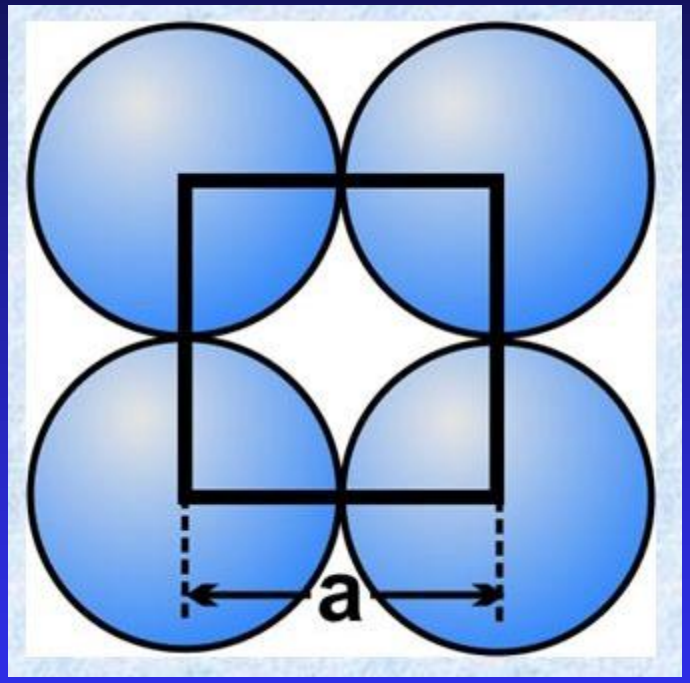
Grado de ocupación sistema CS

$$G.O. = \frac{V_{ocupado\ átomos}}{V_{celda}} = \frac{n_{átomos/celda}\, V_{átomo}}{V_{celda}}$$

$$V_{atómico} = 4/3 \cdot \pi \cdot r^3$$

$$G.O. = \frac{1 \cdot \frac{4}{3} \cdot \pi \cdot \left(\frac{a}{2}\right)^3}{a^3} = \frac{\pi}{6} = \underline{0{,}52\ (52\%)}$$

Área asociada a cada átomo CS

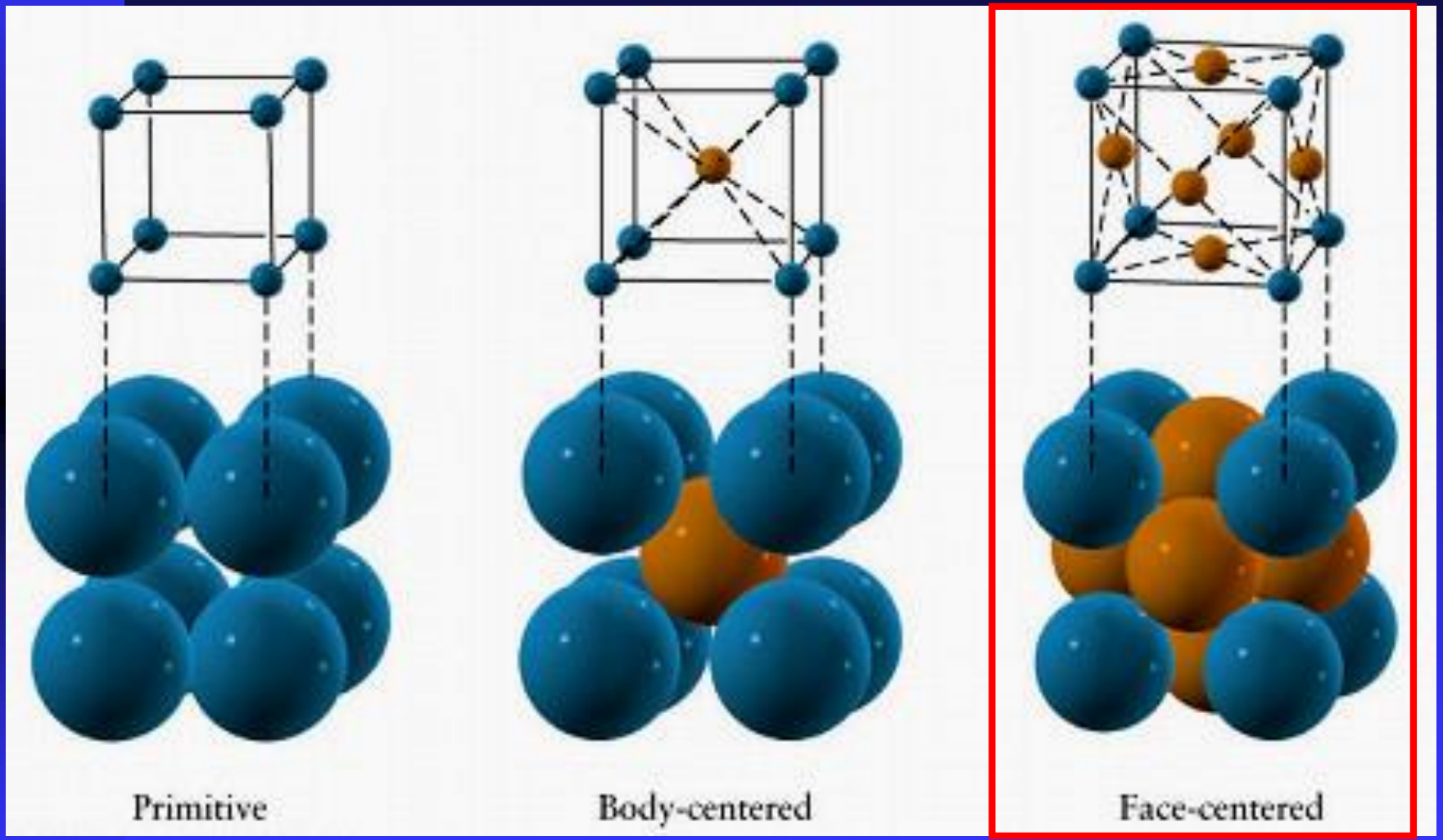


Atomos = 4 . ¼ = 1

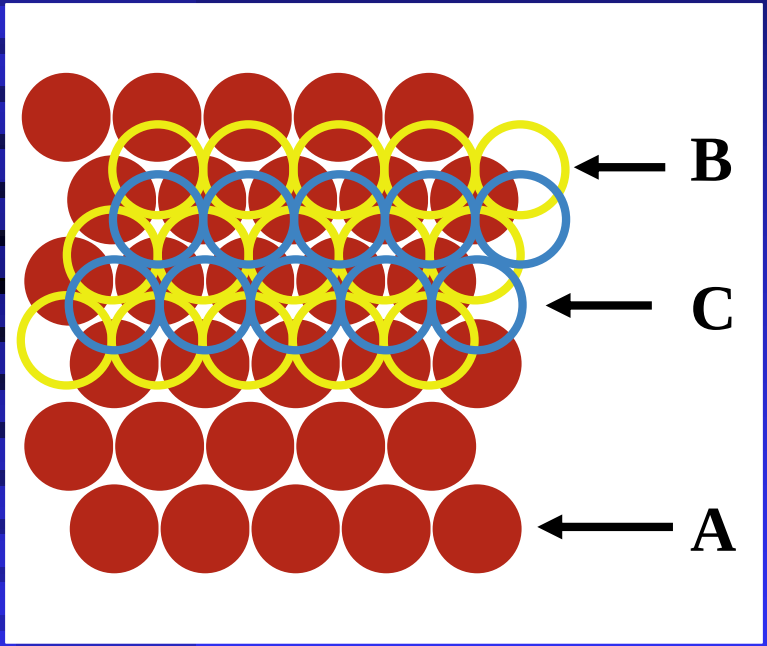
Area = a^2

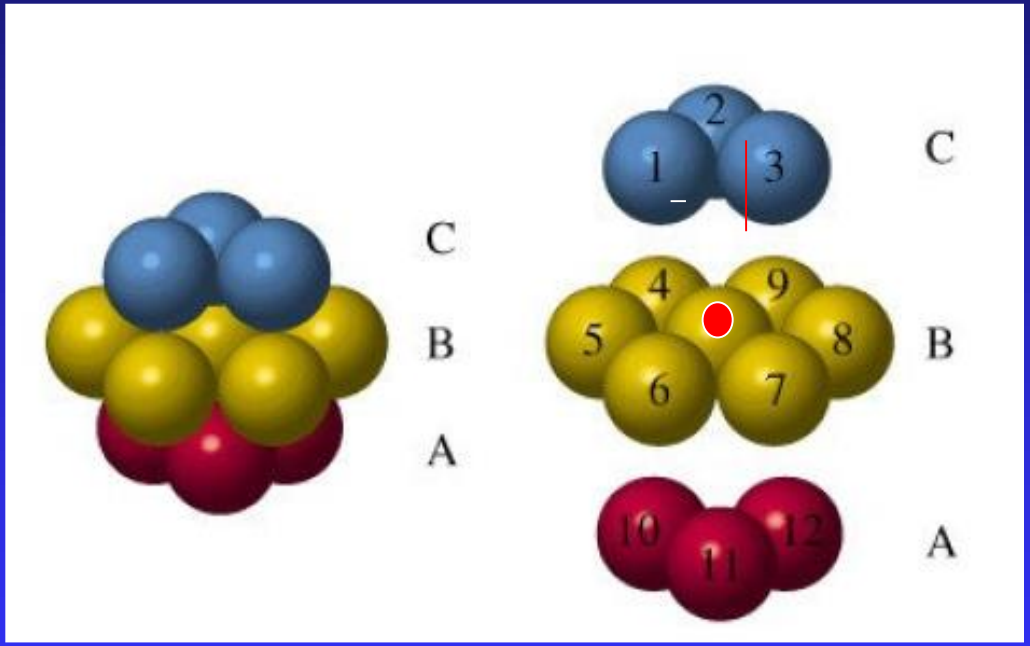
Área asociada a cada átomo = a^2

RED CUBICA

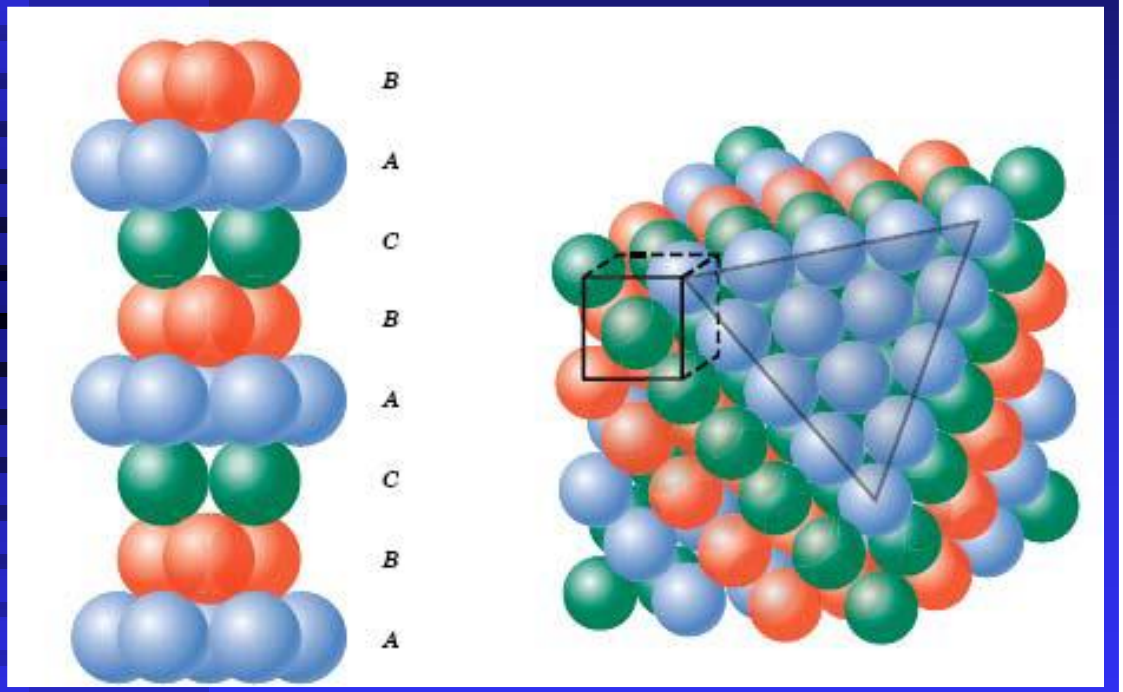


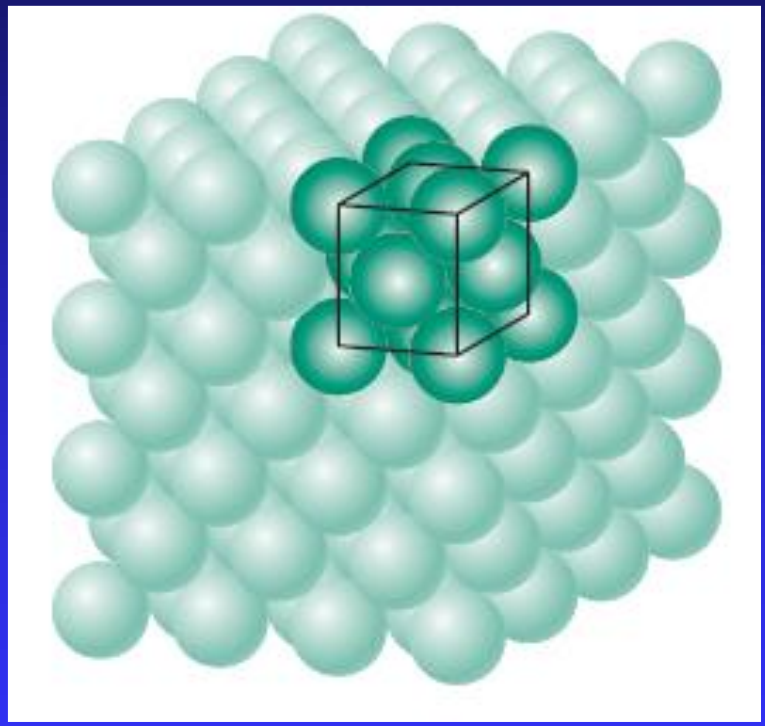
Empaquetamiento compacto ABCABC



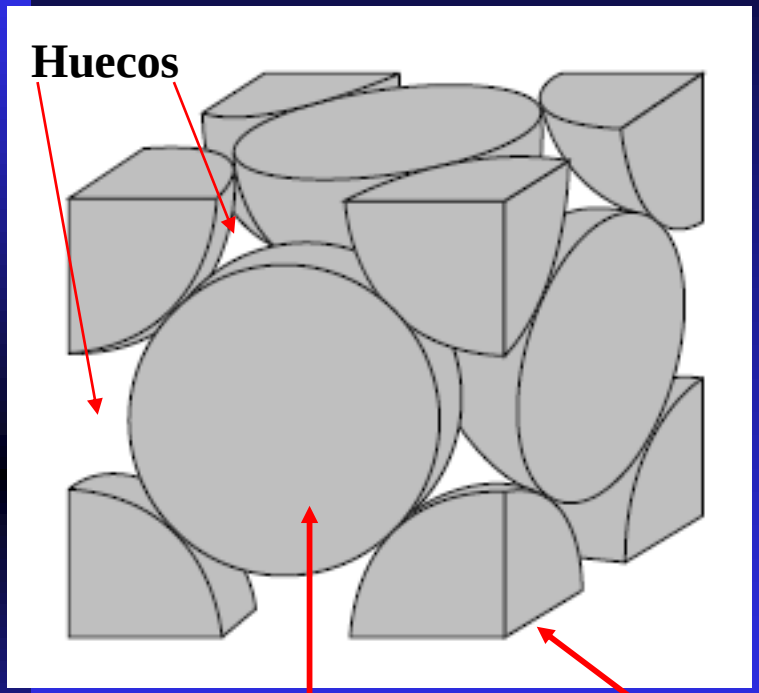


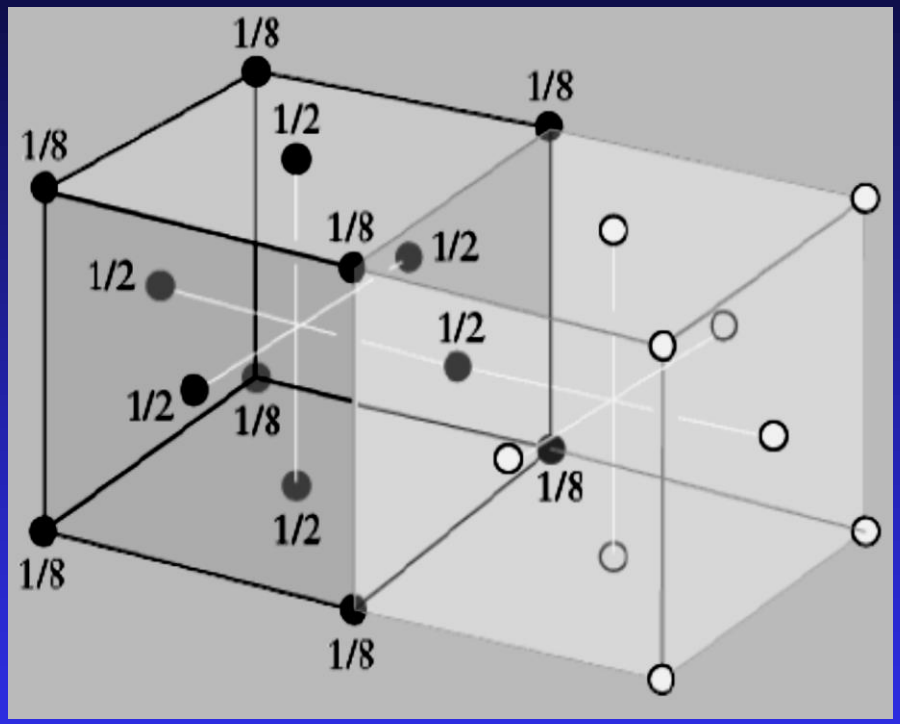
CELDA FCC (Empaquetamiento ABCABC)





Celda cúbica centrada en las caras (FCC)





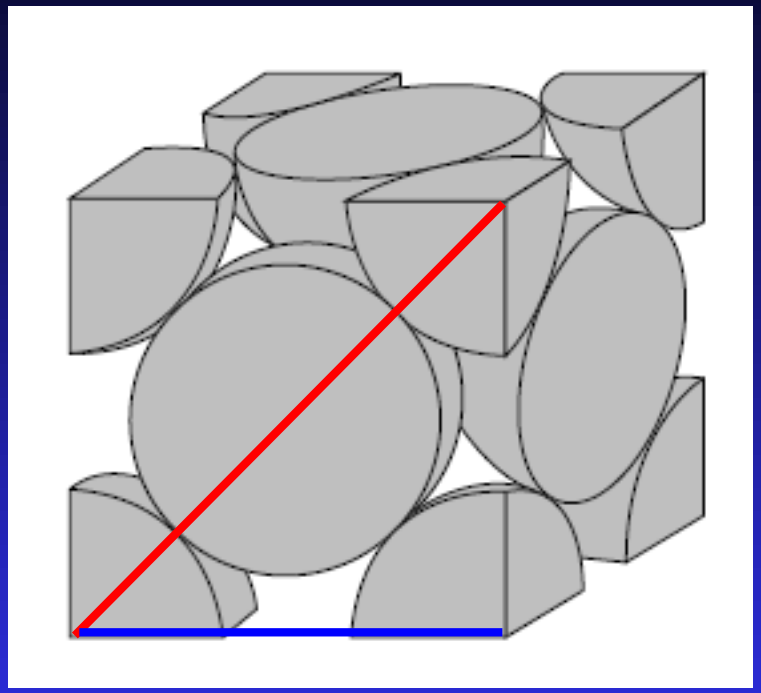
6 . 1/2 = <u>3 átomos</u> por las caras

8 . 1/8 = <u>1 átomo</u> por los vértices

<u>4 átomos / celda</u>

Cristalizan en este sistema: Fe γ, Al, Cu, Pb, Ni, Ag, Au

Relación a/r en celda FCC



Laboratorio de Metalotecnia
ETSIMO

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

$$\left(\frac{a}{r}\right) = 2\sqrt{2} = 2{,}828$$

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

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

Densidad de materiales FCC

$$\rho_{material} = \frac{M_{atómica}}{V_{celda}} = \frac{n_{átomos} \cdot P_{atómico} / N}{(a_{celda})^3}$$

$$\rho = \frac{4\left(P_a / N\right)}{a^3}$$

$P_{a\ metal}$: Tabla I.9, pág. 62

a_{metal} : Tabla I.10, pág. 64

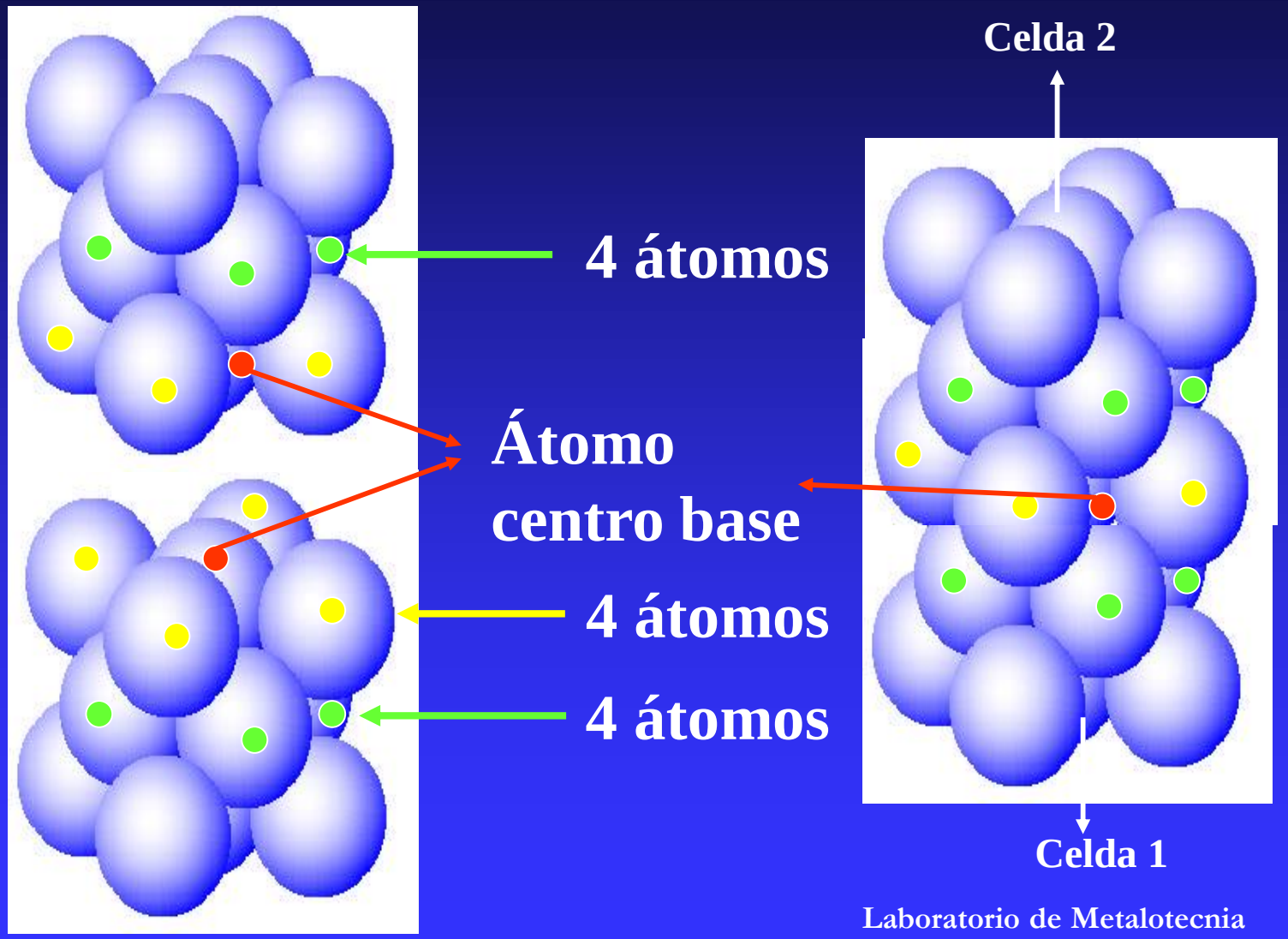
Densidad del Aluminio (FCC)

$P_{a\,Al}$ = 26,98 g/mol (Tabla I.9)

a_{Al} = 4,05 Å (Tabla I.10)

$$\rho_{Al} = \frac{(4\,\text{átomos}.26{,}98\,\text{g}/\text{mol}).(1\text{mol}/6{,}023.10^{23}\,\text{átomos})}{(4{,}05.10^{-8}\,\text{cm})^3} = 2{,}7\,\text{g}/\text{cm}^3$$

Indice de coordinación 12 para sistemas FCC



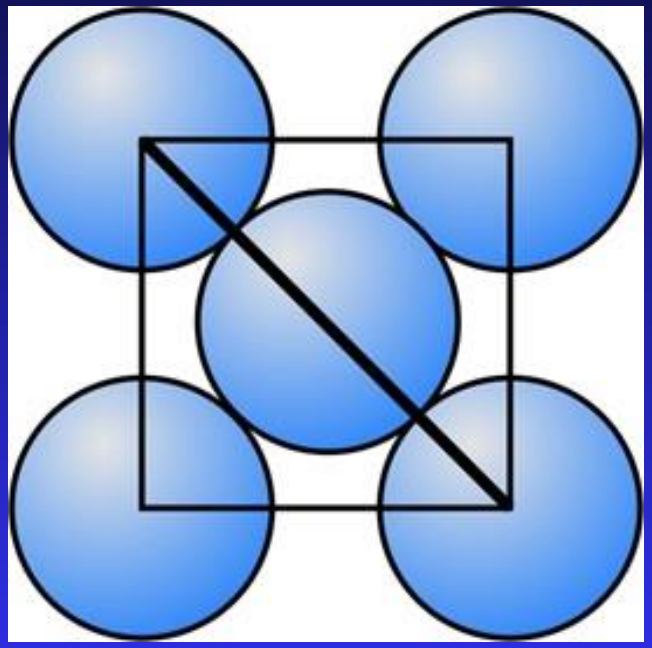
Grado de ocupación sistema FCC

$$G.O. = \frac{V_{ocupado\,átomos}}{V_{celda}} = \frac{n_{átomos}\,V_{átomo}}{V_{celda}}$$

$$V_{atómico} = 4/3 \,.\, \pi \,.\, r^3$$

$$f_{llenado} = \frac{4 \,.\, 4/3\,\pi(a\sqrt{2}/4)^3}{a^3} = \frac{\sqrt{2}}{6} \,.\, \pi = \underline{0{,}74\,(74\%)}$$

Área asociada a cada átomo FCC

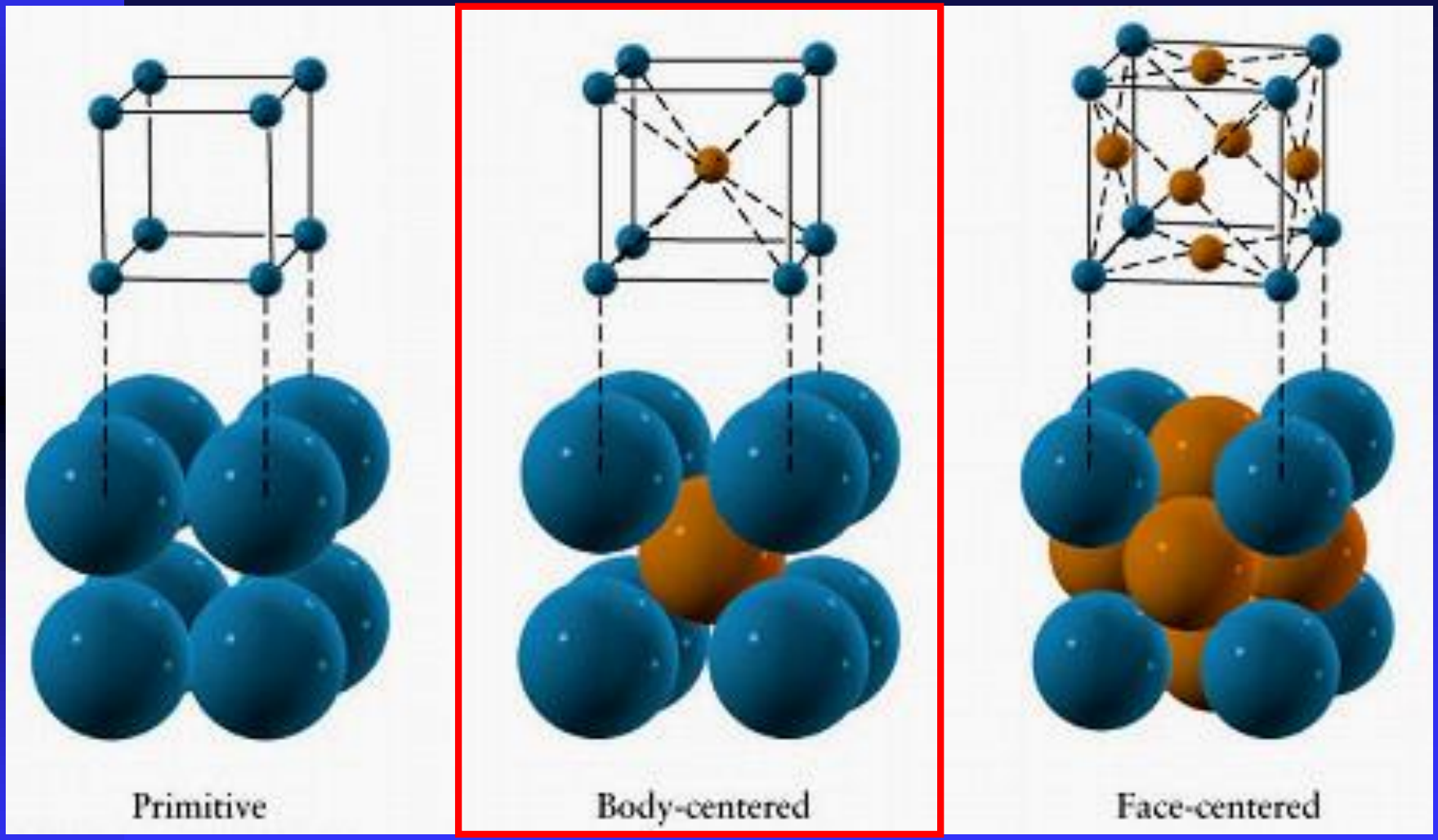


Atomos = (4 . ¼) + 1 = 1 + 1 = 2

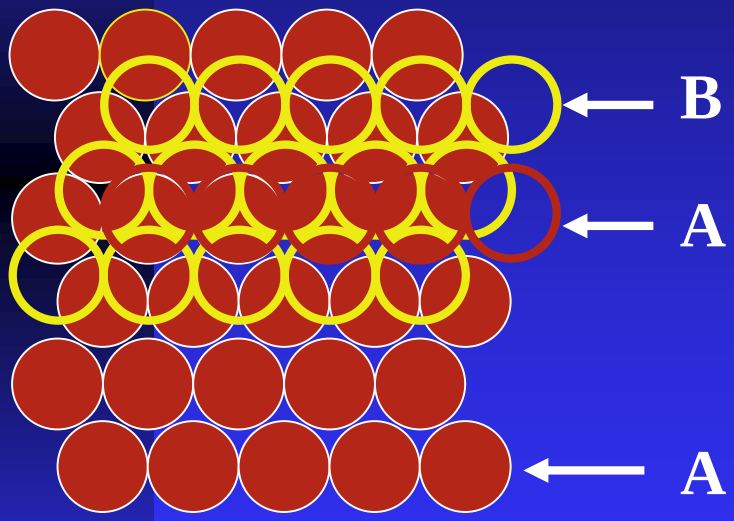
Area = a^2

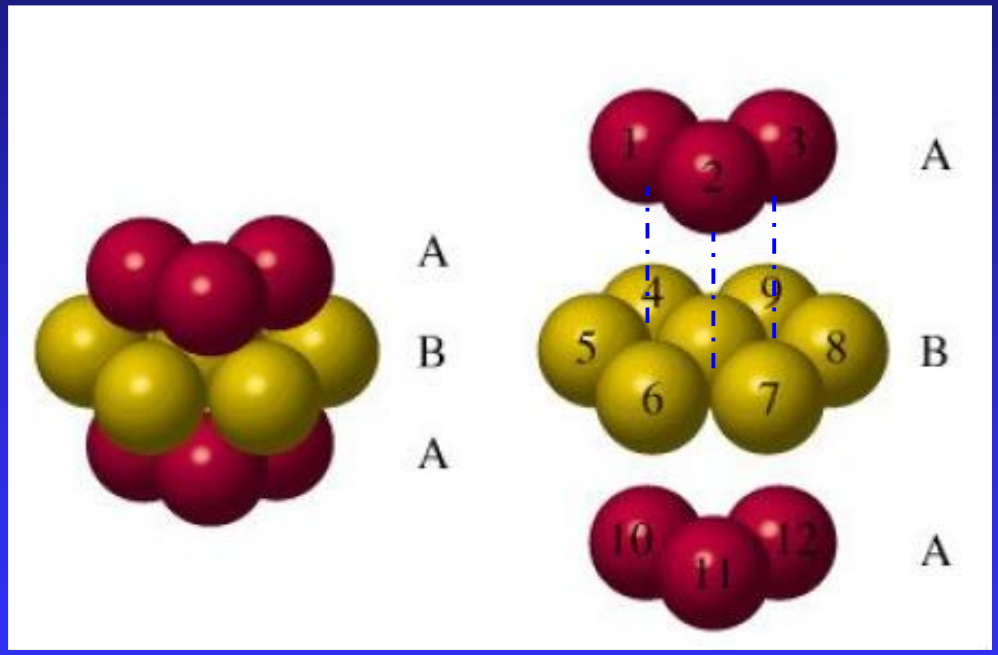
Área asociada a cada átomo = $a^2/2$

RED CUBICA

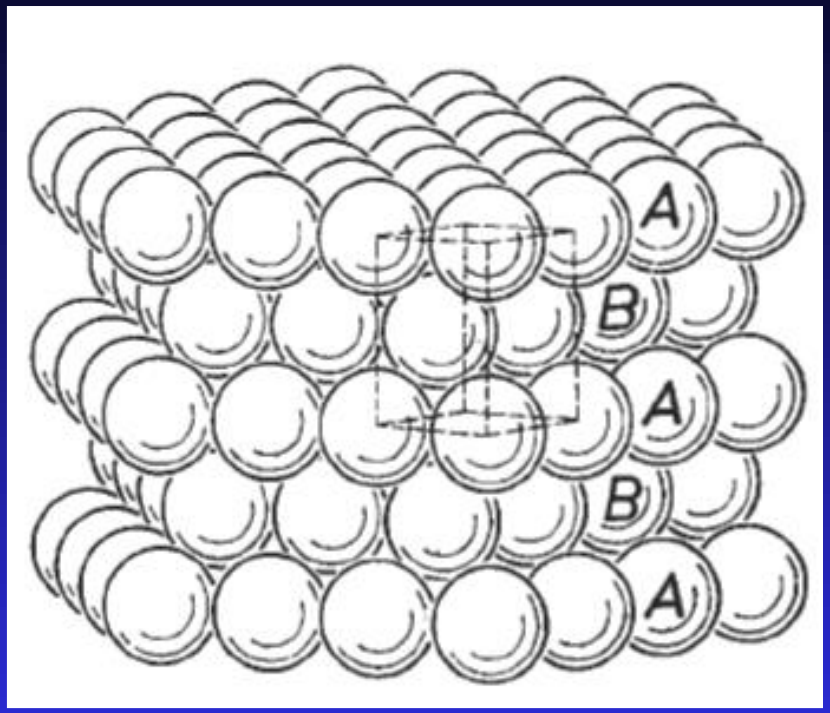


Empaquetamiento compacto ABAB

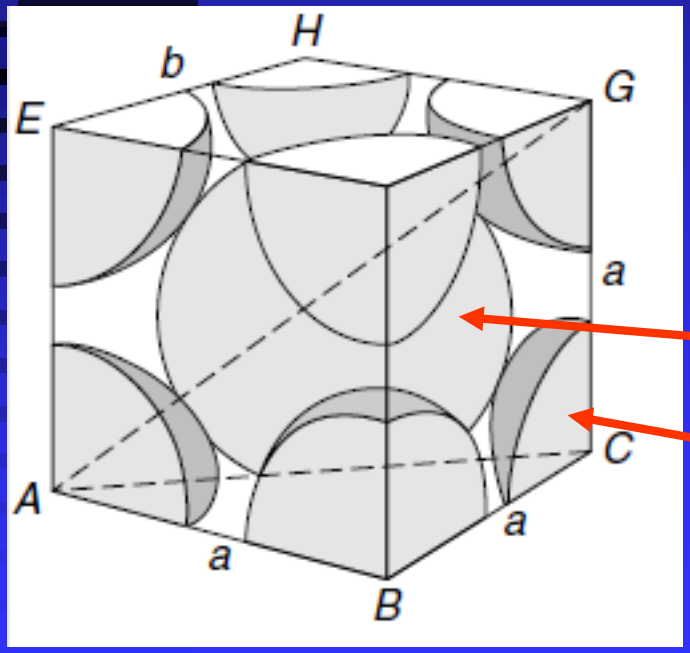




Celda cúbica centrada en el cuerpo (BCC)



Laboratorio de Metalotecnia
ETSIMO



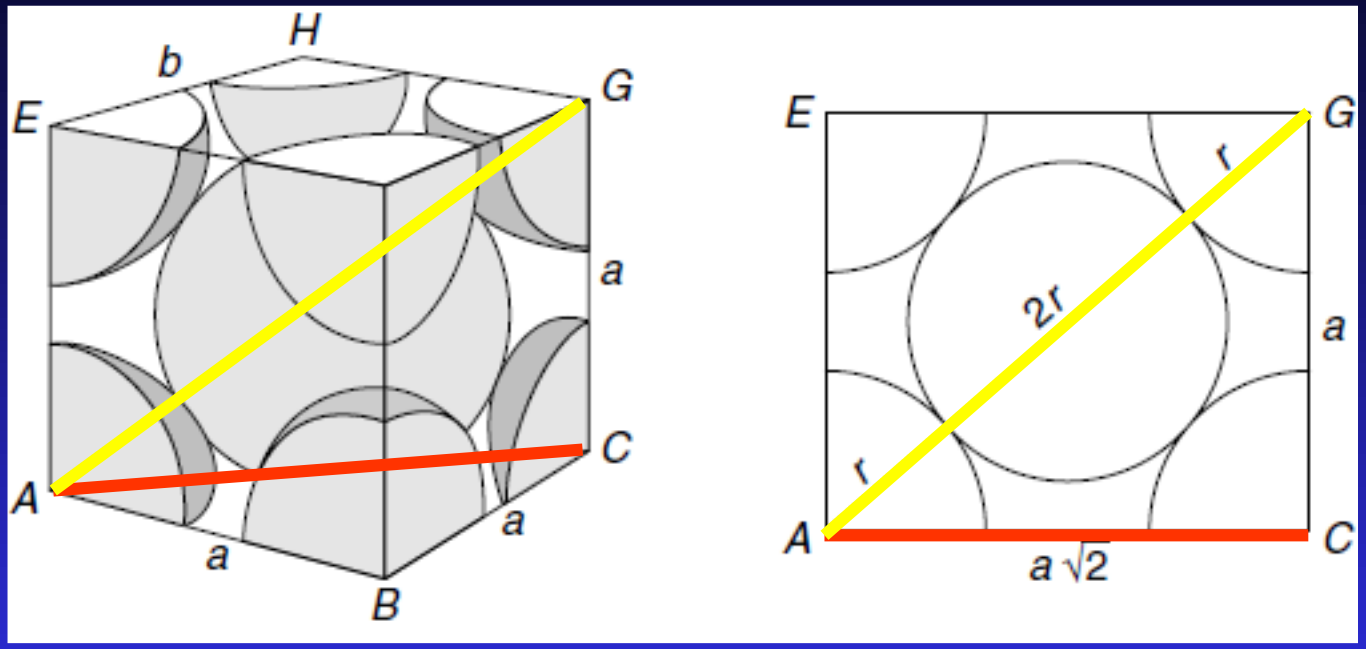
1 átomo centro de la celda

8 . 1/8 = 1 átomo por los vértices

2 átomos / celda

Cristalizan en este sistema: Fe α, V, Cr, Nb, Mo, W

Relación a/r en celda BCC



$$(d)^2 = a^2 + (a\sqrt{2})^2 = 3a^2 \Rightarrow d = 4r = a\sqrt{3}$$

$$\left(\frac{a}{r}\right) = \left(\frac{4\sqrt{3}}{3}\right) = 2{,}309$$

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

Densidad de materiales BCC

$$\rho_{material} = \frac{M_{atómica}}{V_{celda}} = \frac{n_{átomos} \cdot P_{atómico} / N}{(a_{celda})^3}$$

$$\rho = \frac{2\left(P_a / N\right)}{a^3}$$

$P_{a\ metal}$: Tabla I.9, pág. 62

a_{metal} : Tabla 1.10, pág. 64

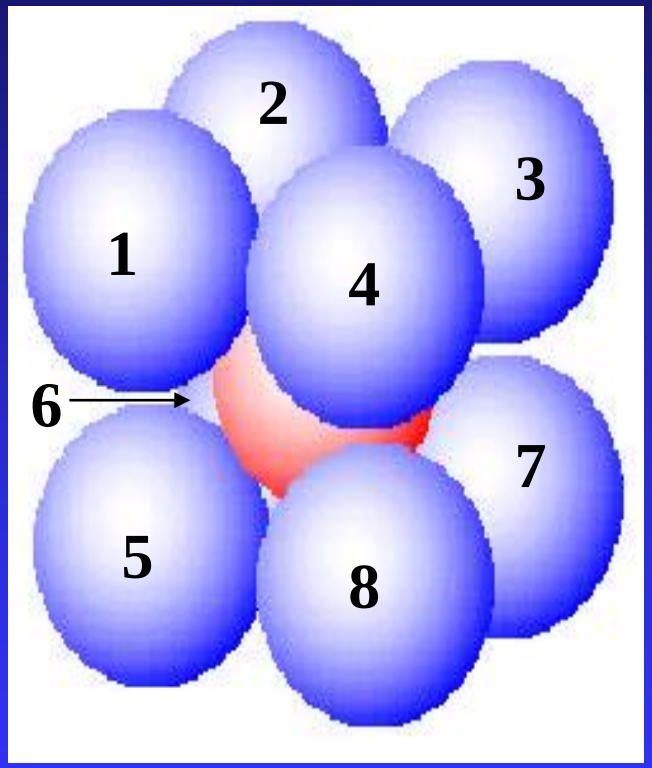
Densidad del Fe α (BCC)

$P_{a\ Fe\ \alpha}$ = 55,847 g/mol (Tabla I.9)

$a_{Fe\ \alpha}$ = 2,8664 Å (Tabla I.10)

$$\rho_{Fe_\alpha} = \frac{(2\ \text{átomos}.\ 55{,}847\ \text{g}/\text{mol}).(1\text{mol}/6{,}023.10^{23}\ \text{átomos})}{(2{,}8664.10^{-8}\ \text{cm})^3} = \underline{7{,}87\ \text{g}/\text{cm}^3}$$

Índice de coordinación 8 para sistemas BCC



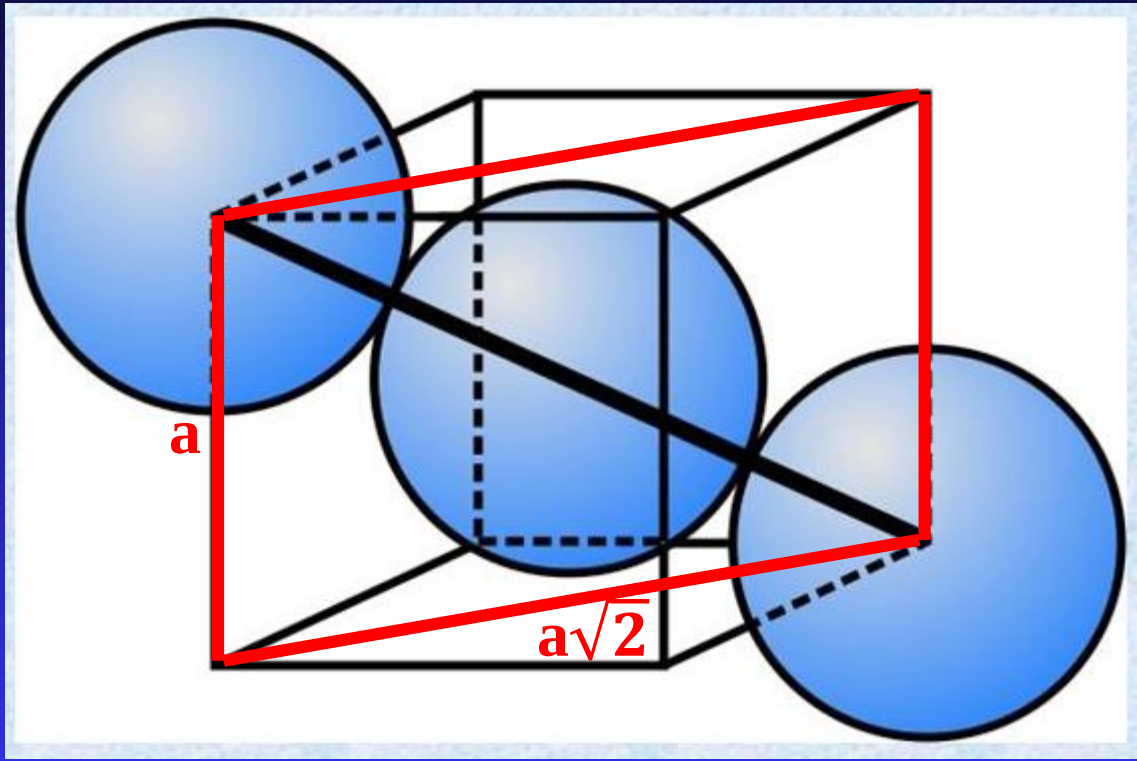
Grado de ocupación sistema BCC

$$G.O. = \frac{V_{ocupado\ átomos}}{V_{celda}} = \frac{n_{átomos} \cdot V_{átomo}}{V_{celda}}$$

$$V_{átomo} = 4/3 \cdot \pi \cdot r^3$$

$$G.O. = \frac{2 \cdot 4/3\,\pi (a\sqrt{3}/4)^3}{a^3} = \frac{\sqrt{3}}{8} \cdot \pi = \underline{0{,}68\ (68\%)}$$

Área asociada a cada átomo BCC



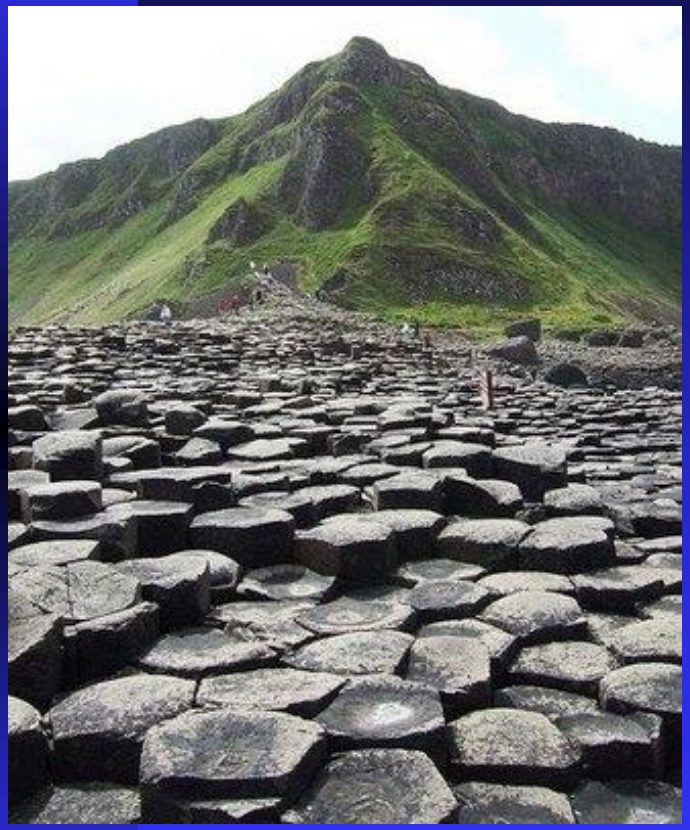
Atomos = 4 . ¼ + 1 = 1 + 1 = 2

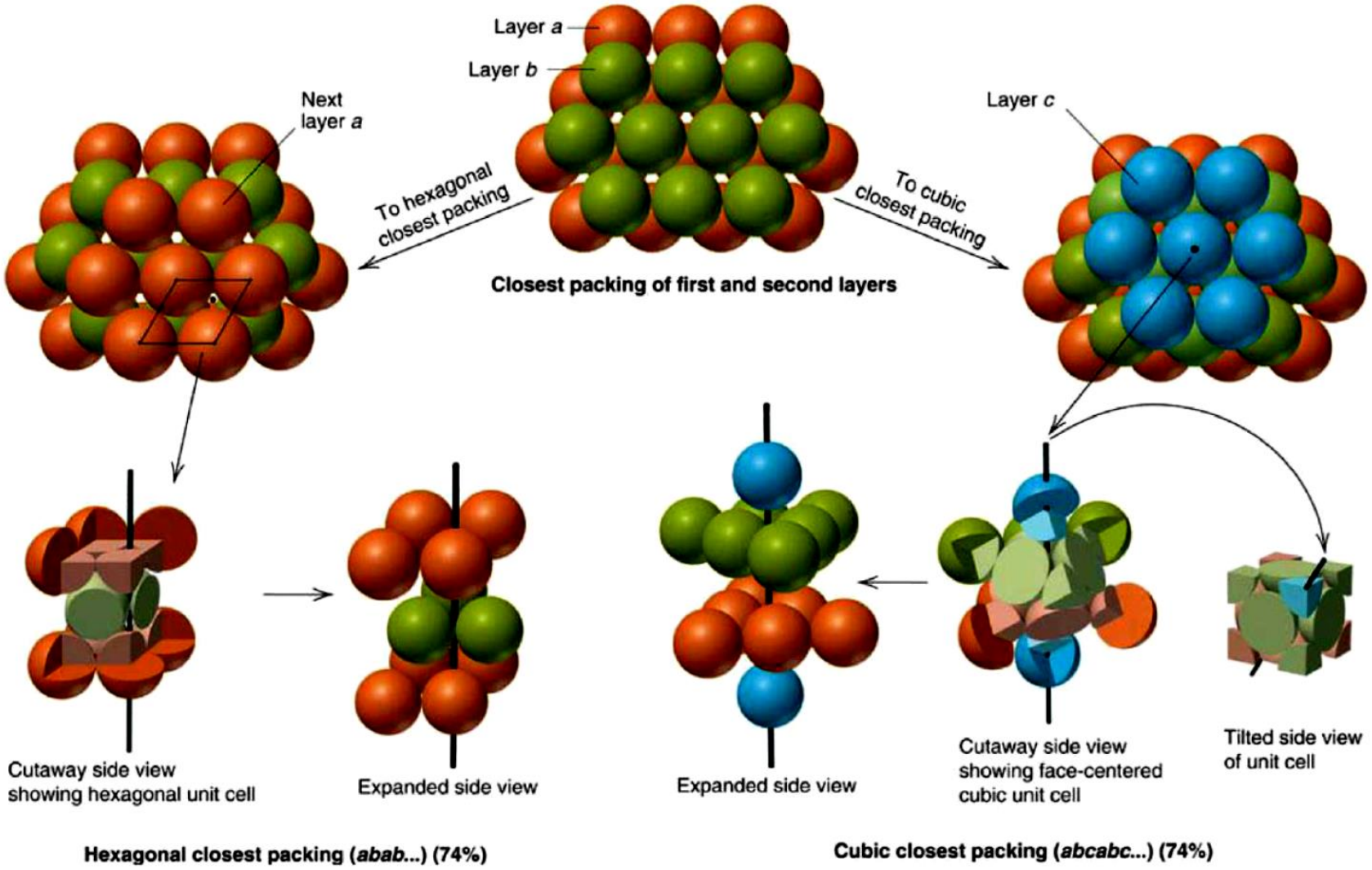
Area = $a \cdot a\sqrt{2} = a^2\sqrt{2}$

Área asociada a cada átomo = $a^2\sqrt{2}/2$

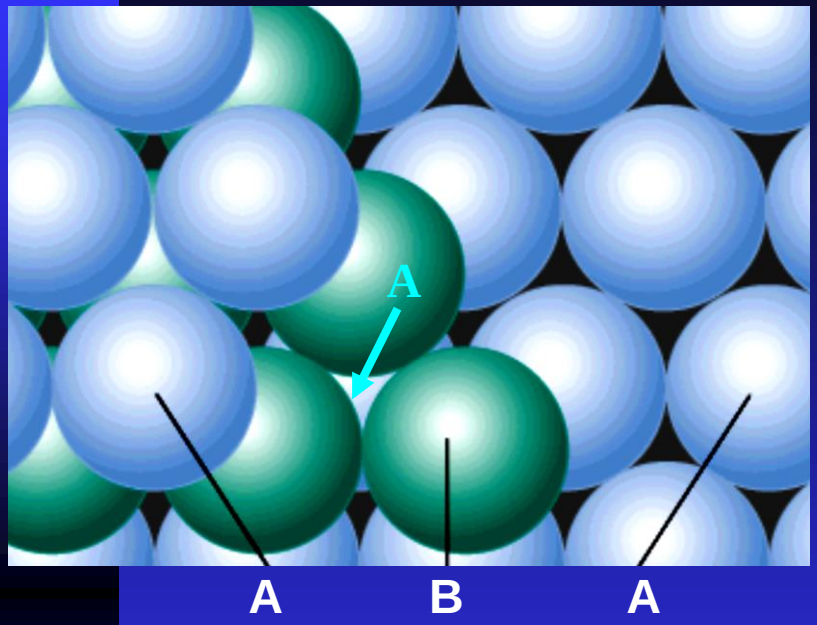
	FCC	BCC
Índice coordinación	12	8
Átomos / celda	4	2
Relación a / r	2,828	2,309
Volumen atómico	$4 \cdot 4/3\ \pi r^3$	$2 \cdot 4/3\ \pi r^3$
Volumen celda	$\left(4r/\sqrt{2}\right)^3$	$\left(4r/\sqrt{3}\right)^3$
Fracción de llenado	0,74	0,68

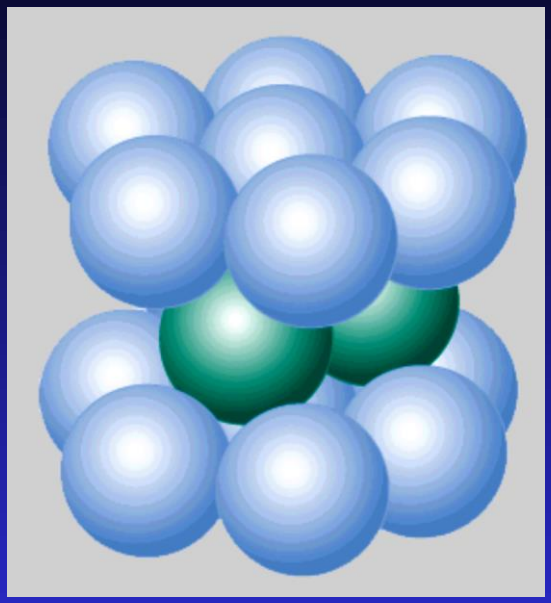
Empaquetamiento hexagonal compacto



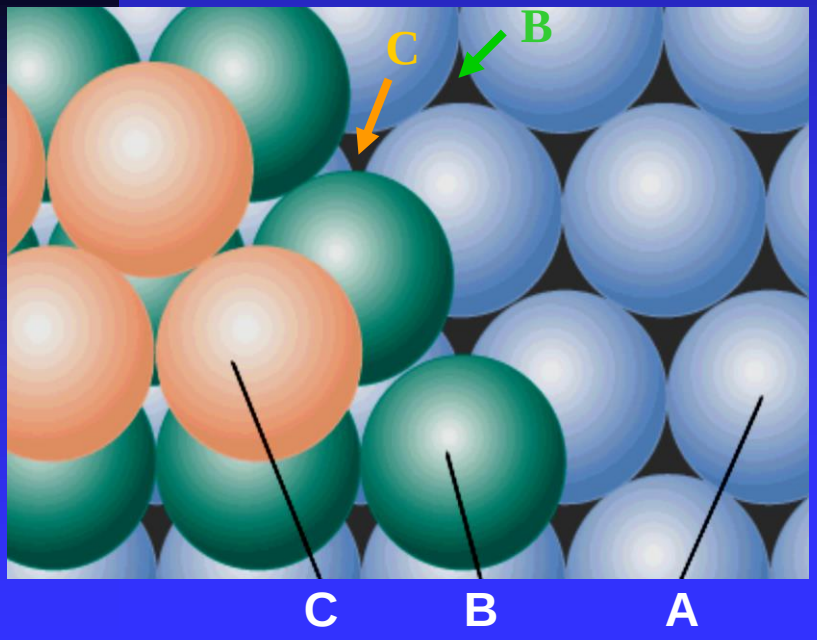

Layer a
Layer b
Next layer a
Layer c
To hexagonal closest packing
To cubic closest packing
Closest packing of first and second layers
Cutaway side view showing hexagonal unit cell
Expanded side view
Expanded side view
Cutaway side view showing face-centered cubic unit cell
Tilted side view of unit cell
Hexagonal closest packing (abab...) (74%)
Cubic closest packing (abcabc...) (74%)

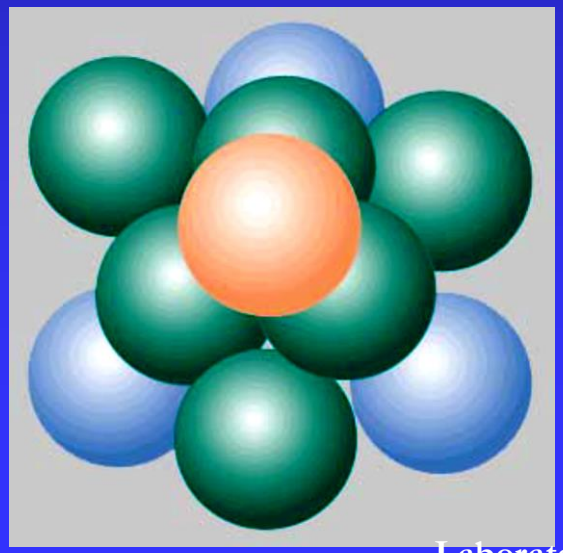
EMPAQUETAMIENTO COMPACTO





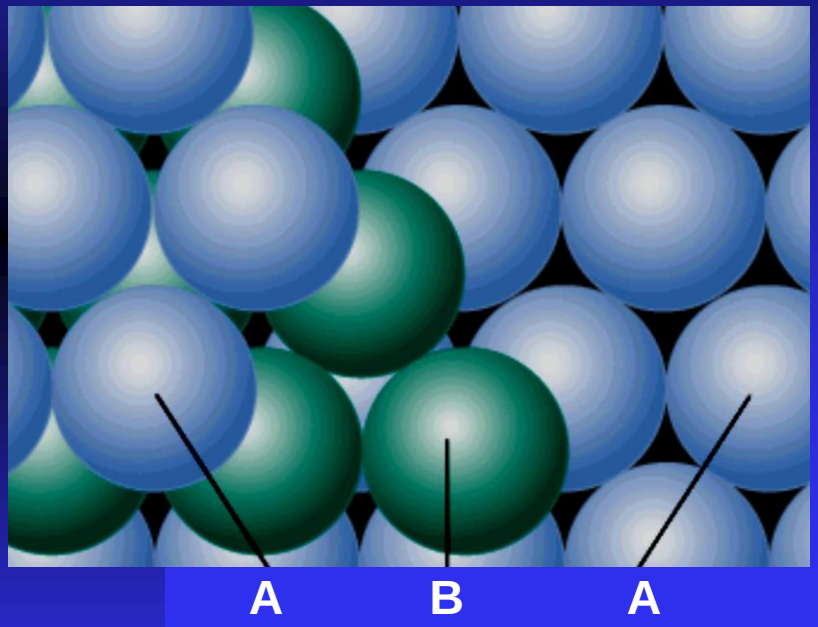
HC

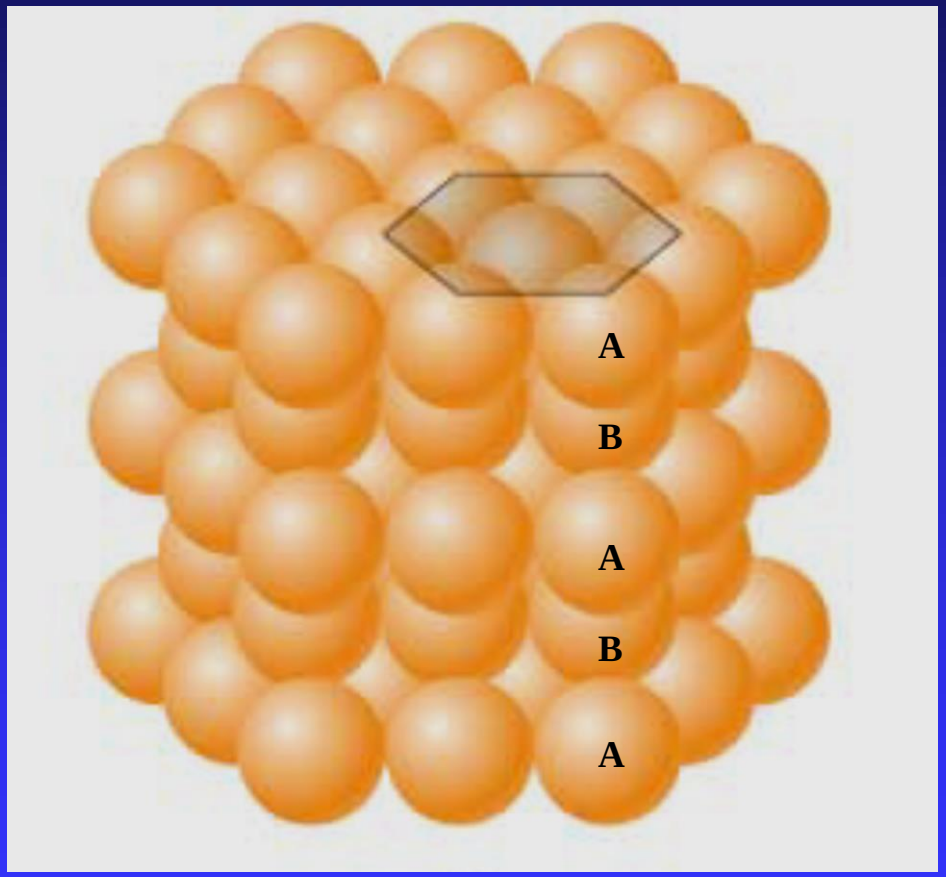




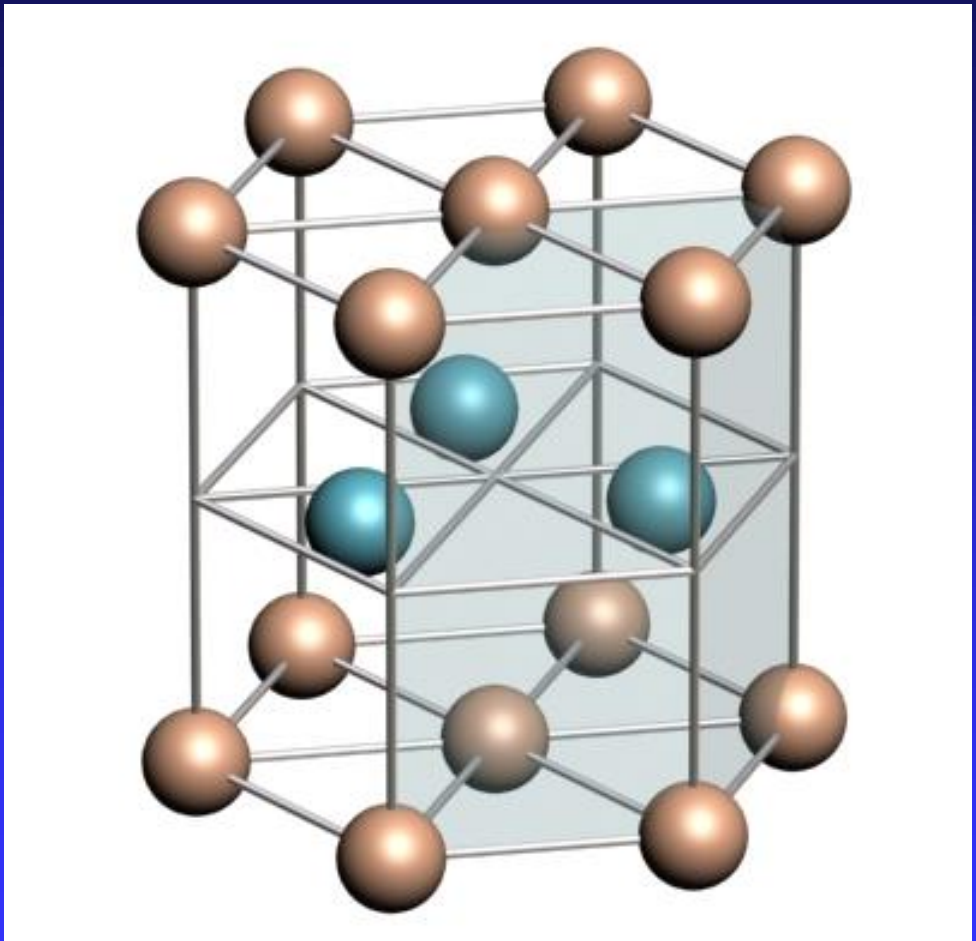
FCC

Celda Hexagonal (Empaquetamiento ABAB)

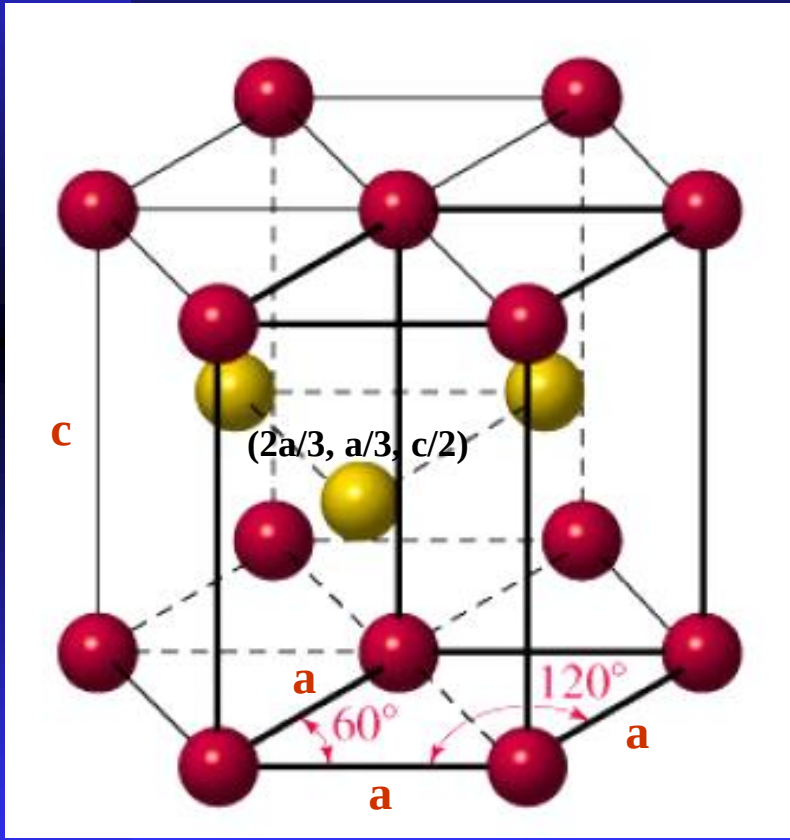


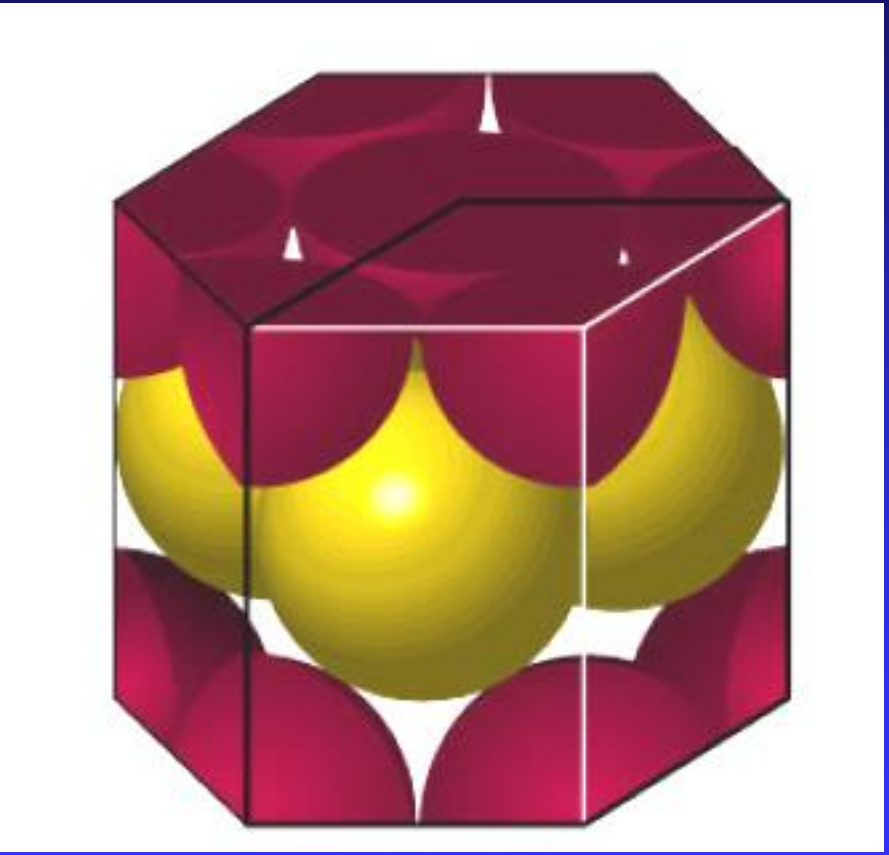


Celda Hexagonal (Empaquetamiento ABAB)

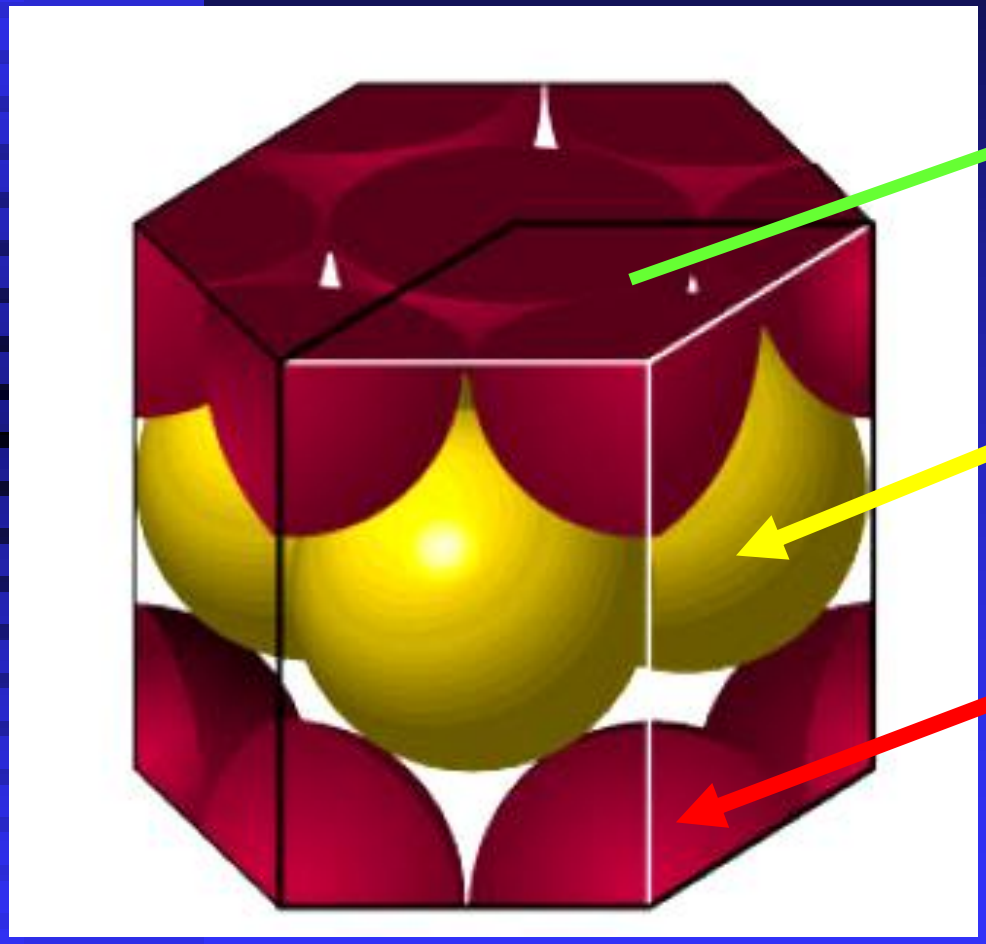


Celda Hexagonal (Empaquetamiento ABAB)





Celda Hexagonal (Empaquetamiento ABAB)



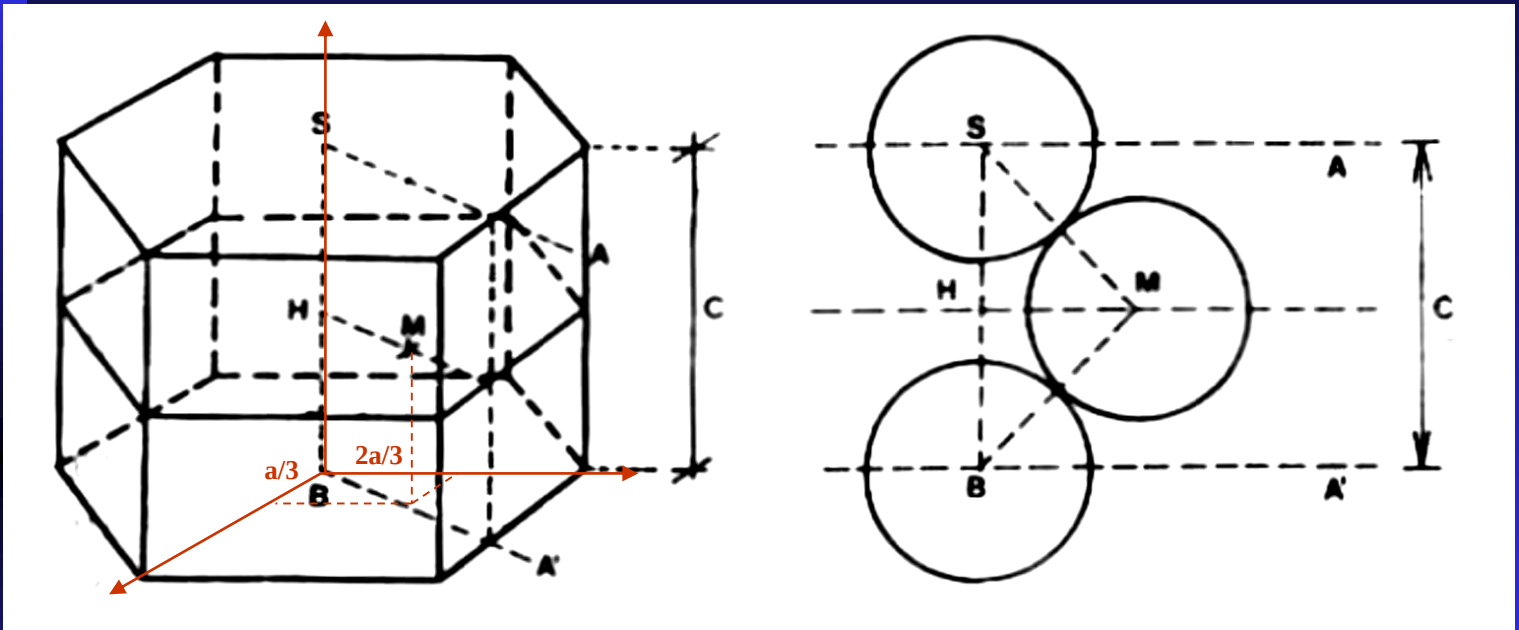
Celda elemental (prisma romboédrico)

1 átomo central

8 . 1/8 = 1 átomo por los vértices

2 átomos / celda

Relación c/a en celda HC



$(2a/3)^2 = MH^2 + (a/3)^2 \rightarrow MH^2 = (2a/3)^2 - (a/3)^2 = (a/3)^2 \rightarrow \underline{MH = a/\sqrt{3}}$

$MH^2 = MB^2 - HB^2 = a^2 - (c/2)^2$

$(a/\sqrt{3})^2 = a^2 - (c/2)^2 \rightarrow a^2/3 = a^2 - (c^2/4);\ c^2/4 = 2a^2/3$

$c^2/a^2 = 8/3;\ c/a = \sqrt{(8/3)} = \underline{1,633}$

Densidad de materiales HC

Partiendo del prisma romboédrico como celda elemental:

$$\rho_{material} = \frac{M_{atómica}}{V_{celda}} = \frac{n_{átomos} \cdot P_{atómico} / N}{(\text{Area base} \cdot c)}$$

$$\rho = 2 \cdot (P_a / N) / [(a^2 \cdot \sqrt{3}/2) \cdot c]$$

$P_{a\ metal}$: **Tabla I.9, pág. 62**

A, c_{metal} : **Tabla 1.10, pág. 64**

Densidad del Magnesio (HC)

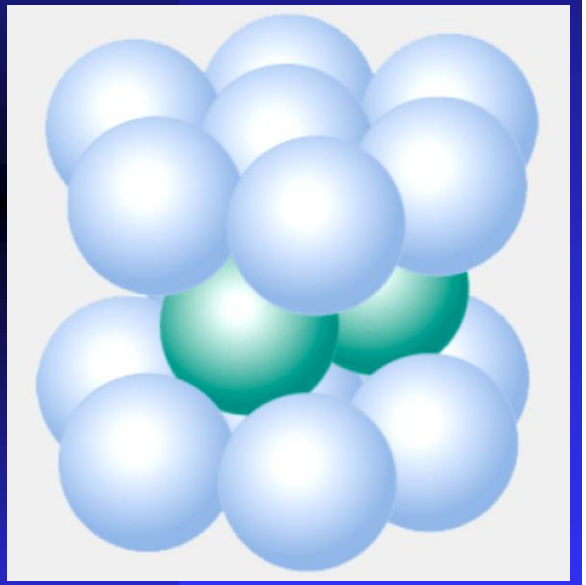
P_a = 24,305 g/mol (Tabla I.9)

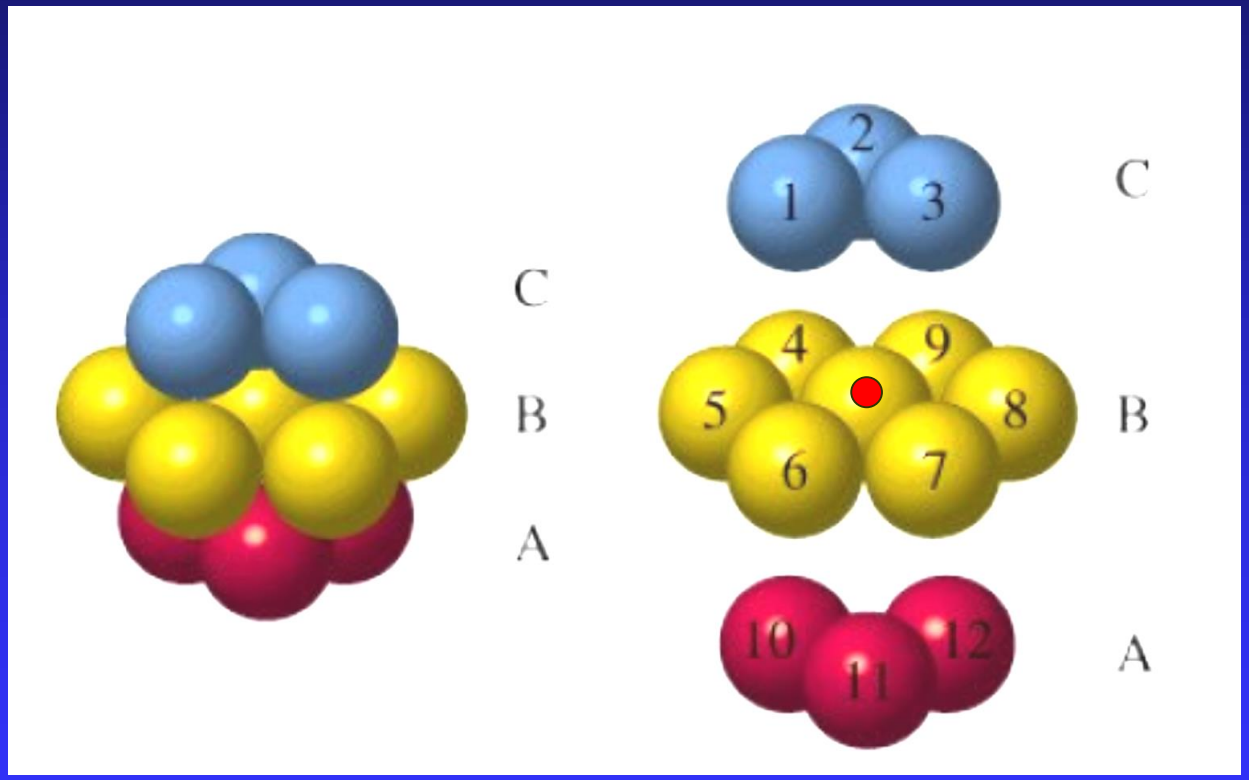
a = 3,2092 Å; c = 5,2103 Å (Tabla I.10)

$$\rho = 2 \cdot (P_a / N) / [(a^2 . \sqrt{3}/2) \cdot c]$$

$$\rho_{Mg} = \frac{(2\ \text{átomos}.24{,}305\ \text{g/mol}) \cdot (1\text{mol}/6{,}023.10^{23}\ \text{átomos})}{(3{,}2092.10^{-8}\ \text{cm})^2 \cdot (5{,}2103.10^{-8}\ \text{cm}) \cdot \sqrt{3}/2} = \underline{1{,}74\ \text{g/cm}^3}$$

Índice coordinación 12 para sistema hexagonal





Grado de ocupación sistema HC

$$G.O. = \frac{V_{ocupado\ átomos}}{V_{celda}} = \frac{n_{átomos} V_{átomo}}{V_{celda}}$$

$$V_{atómico} = 4/3 \cdot \pi \cdot r^3$$

$$V_{prisma} = A_{base} \cdot Altura = [a^2 \sqrt{3} / 2] \cdot c$$

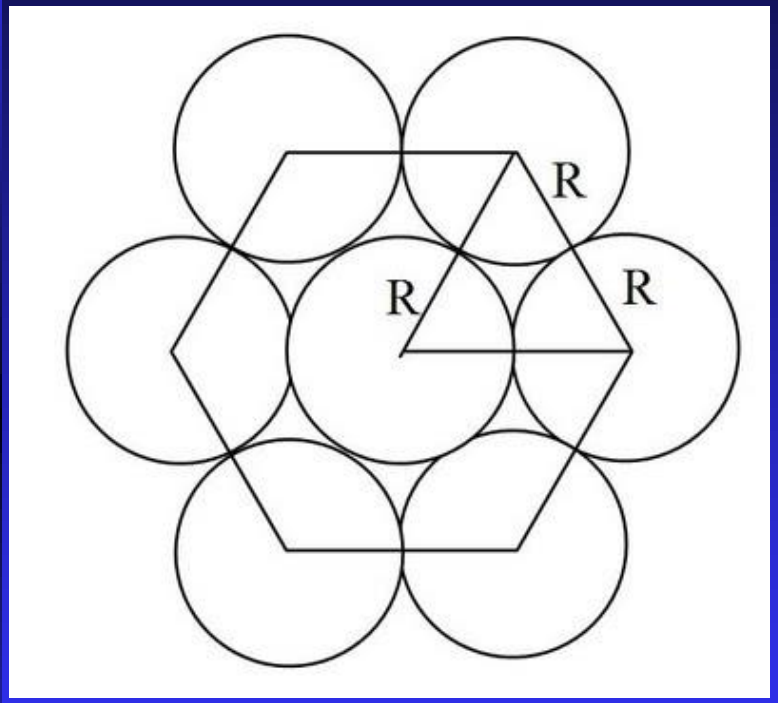
$$c = a \sqrt{8/3}$$

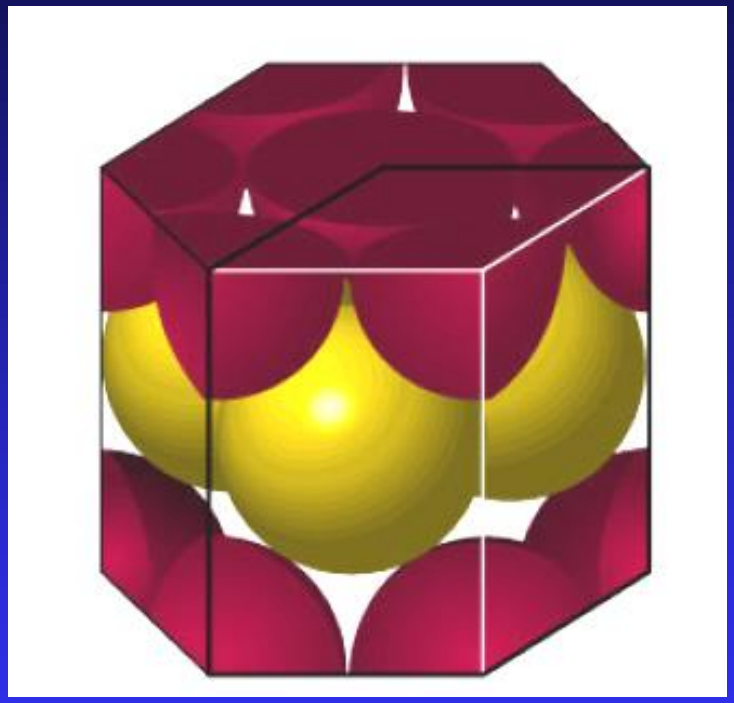
$$V_{celda} = a^2\sqrt{3} /2 \cdot a\sqrt{8/3} = a^3 \sqrt{2}$$

$$G.\ O. = 2 \cdot 4/3\ \pi\ (a/2)^3 / a^3\sqrt{2} = 0{,}74\ (74\%)$$

Área asociada a cada átomo

Base hexagonal





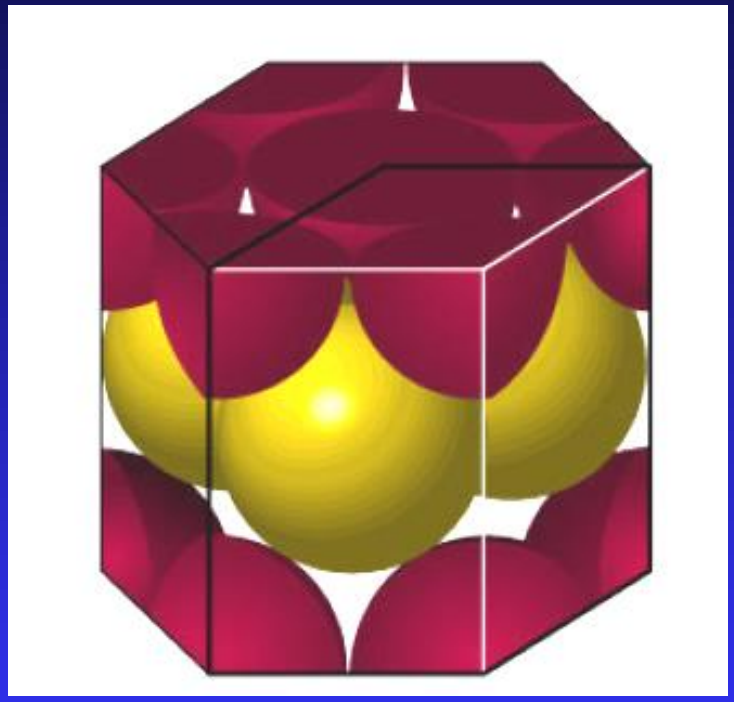
Atomos = 6 . 1/3 + 1 = 3

Area = $3a^2\sqrt{3}/2$

Área asociada a cada átomo = $a^2\sqrt{3}/2$

Área asociada a cada átomo

Base rómbica



Atomos = 4 . ¼ = 1

Area = $a^2 \sqrt{3}$ /2

Área asociada a cada átomo = $a^2\sqrt{3}/2$