

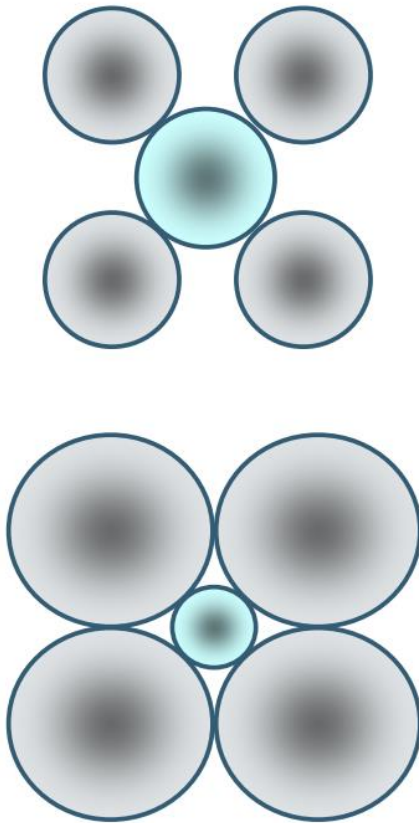
INSERCCIONES OCTAEDRICAS Y TETRAEDRICAS EN REDES FCC Y BCC

INSERCIONES OCTAEDRICAS Y TETRAEDRICAS EN REDES FCC Y BCC

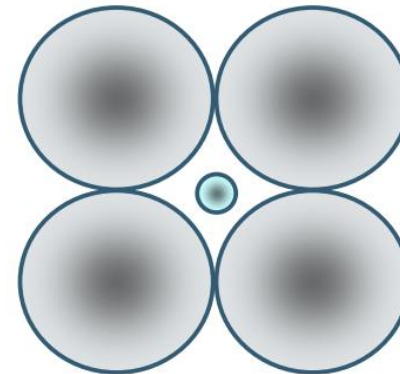
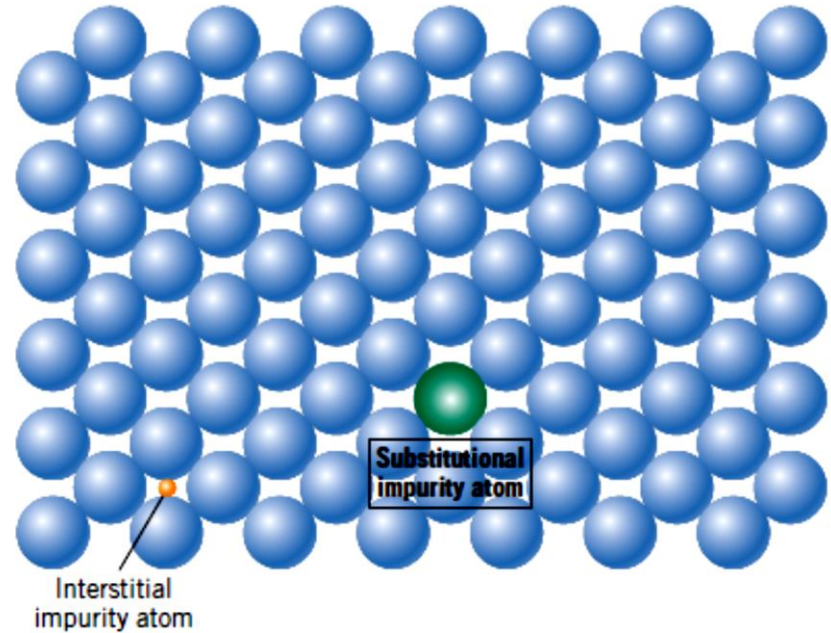
REFERENCIA BIBLIOGRÁFICA:

- **Pp. 110 – 114** “CIENCIA E INGENIERIA DE MATERIALES”. Prof. José Antonio Pero-Sanz Elorz

ATOMOS INTERSTICIALES Y DE SUSTITUCION

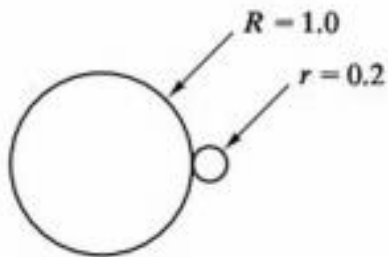


Estables

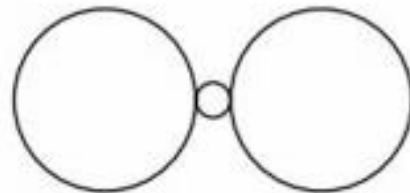


Inestable

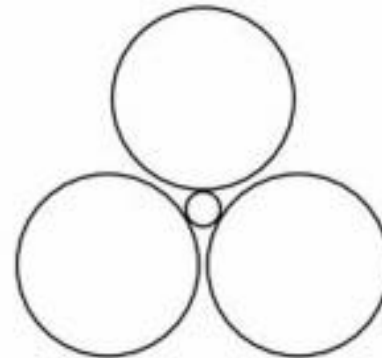
Coordinación entre compuestos iónicos: $r_i/r_s = 0,2$



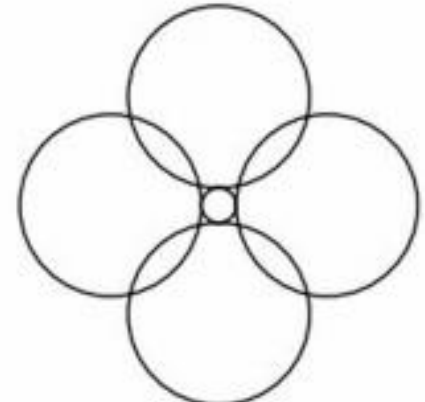
CN = 1 posible



CN = 2 posible



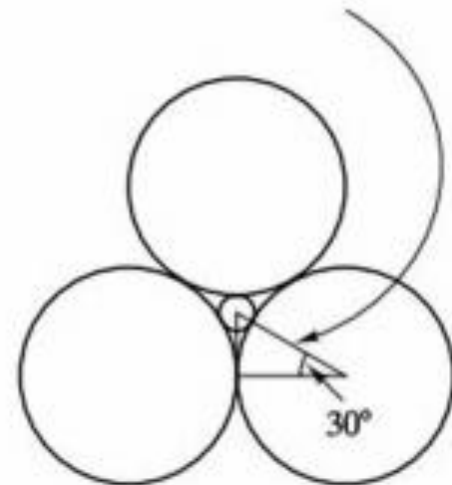
CN = 3 máximo



CN = 4 inestable

Relación $(r_i/r_s)_{\min}$ para una coordinación 3

$$\cos 30^\circ = 0.866 = \frac{R}{r + R} \rightarrow \frac{r}{R} = 0.155$$



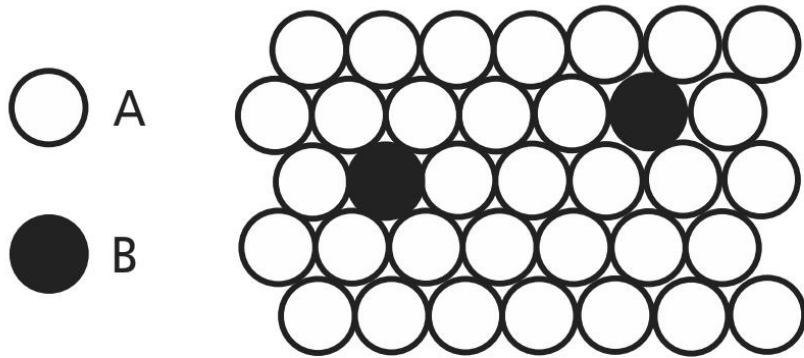


Schéma à deux dimensions
d'une solution solide de substitution de B dans A.

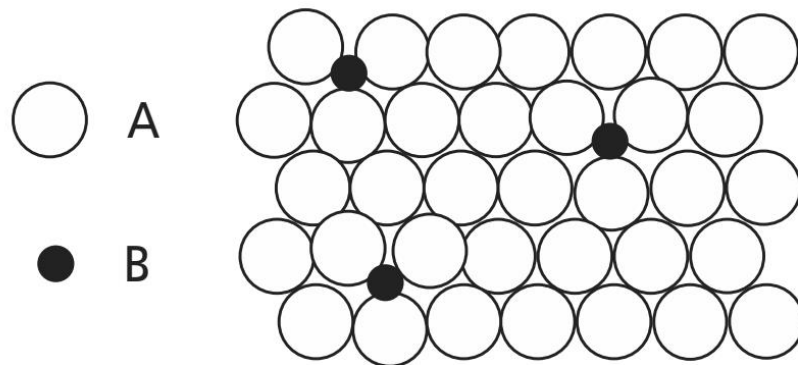




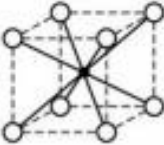
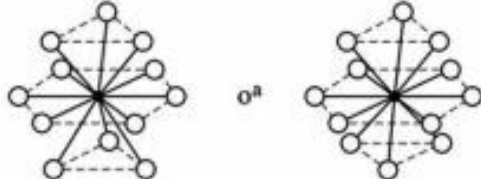


Schéma à deux dimensions
d'une solution solide d'insertion de B dans A.

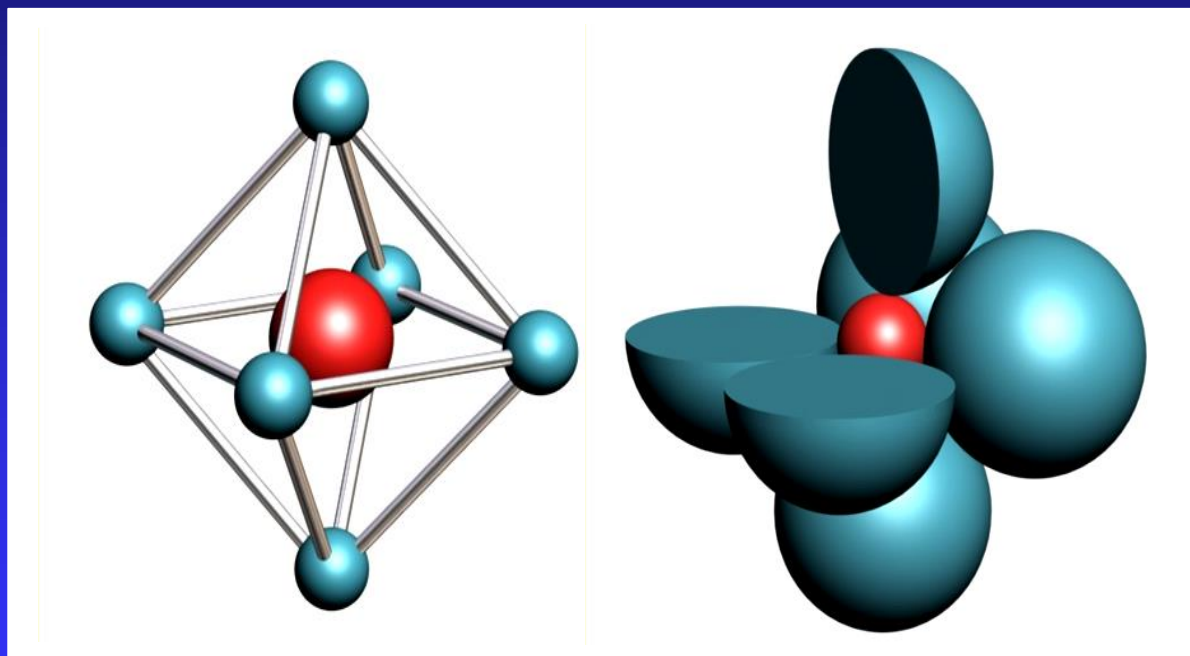
$$\frac{a - a_0}{a_0} = x_B \frac{r_B - r_A}{r_A}$$

Relación de radios anión-cación para huecos

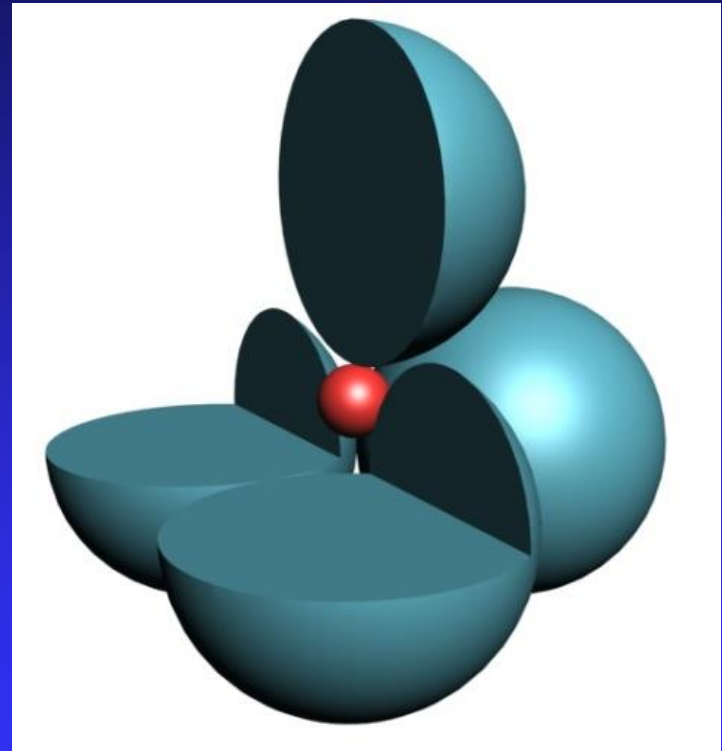
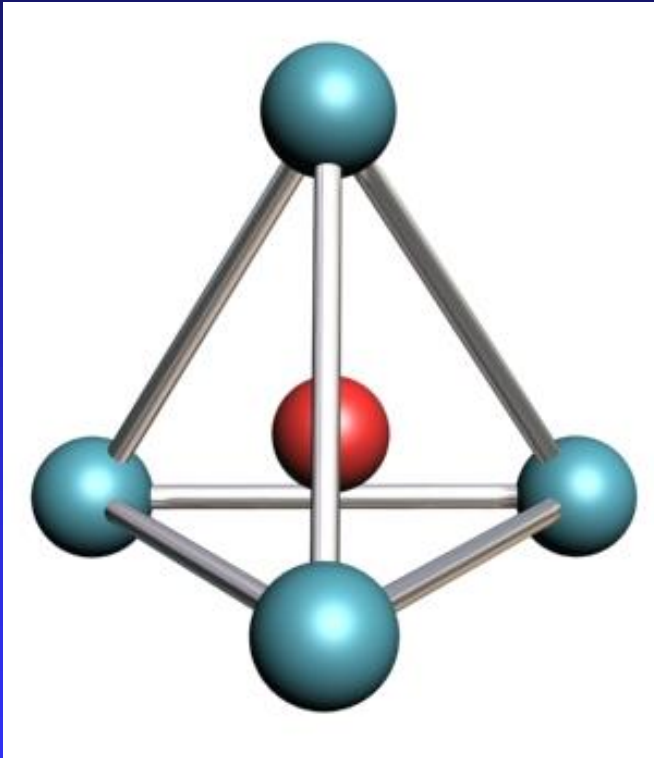
Número de coordinación	Relación entre radios r/R	Geometría de coordinación
2	$0 < \frac{r}{R} < 0.155$	
3	$0.155 \leq \frac{r}{R} < 0.225$	
4	$0.225 \leq \frac{r}{R} < 0.414$	
6	$0.414 \leq \frac{r}{R} < 0.732$	
8	$0.732 \leq \frac{r}{R} < 1$	
12	1	

* La geometría de la izquierda corresponde a la estructura hexagonal compacta (hcp), y la de la derecha a la estructura cúbica centrada en las caras (fcc). Estas estructuras cristalinas se verán en el Capítulo 3.

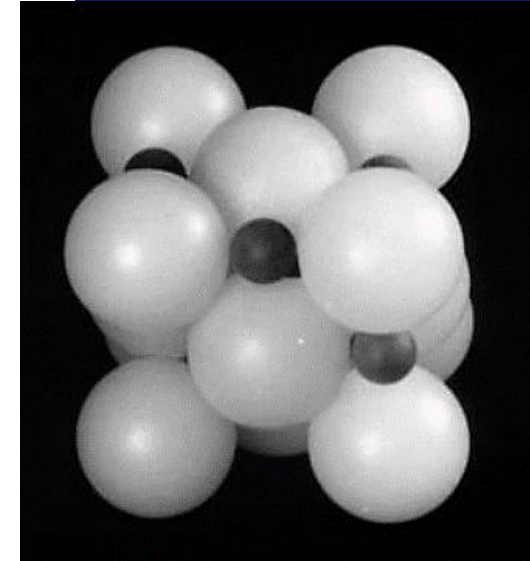
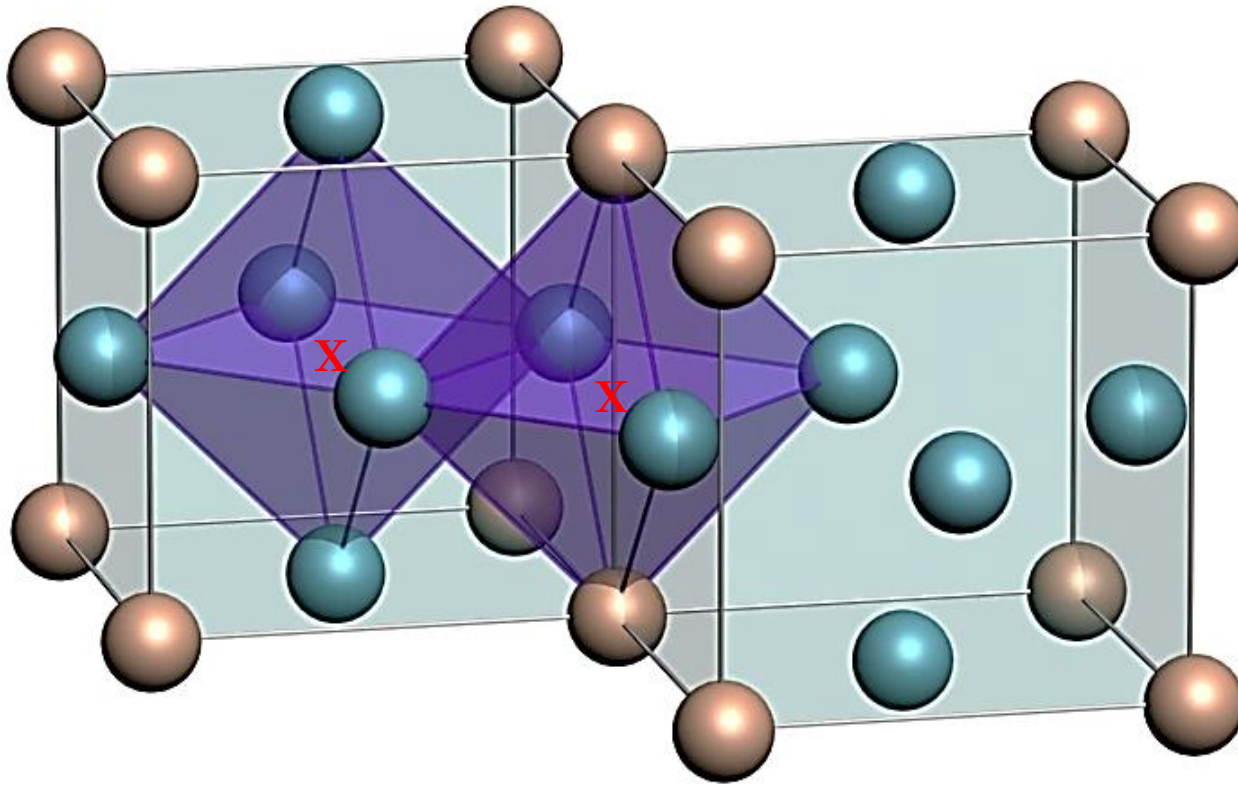
INSERCIONES OCTAEDRICAS



Huecos tetraédricos



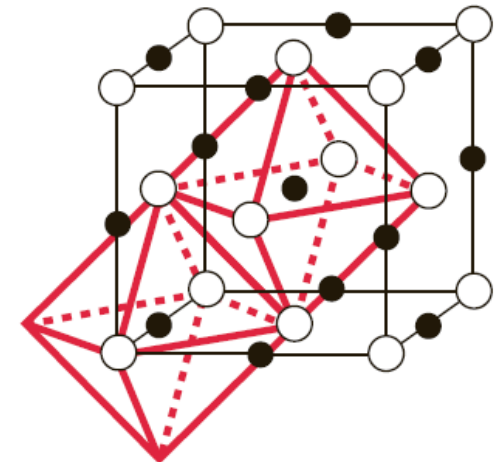
Sistema FCC: Huecos octaédricos



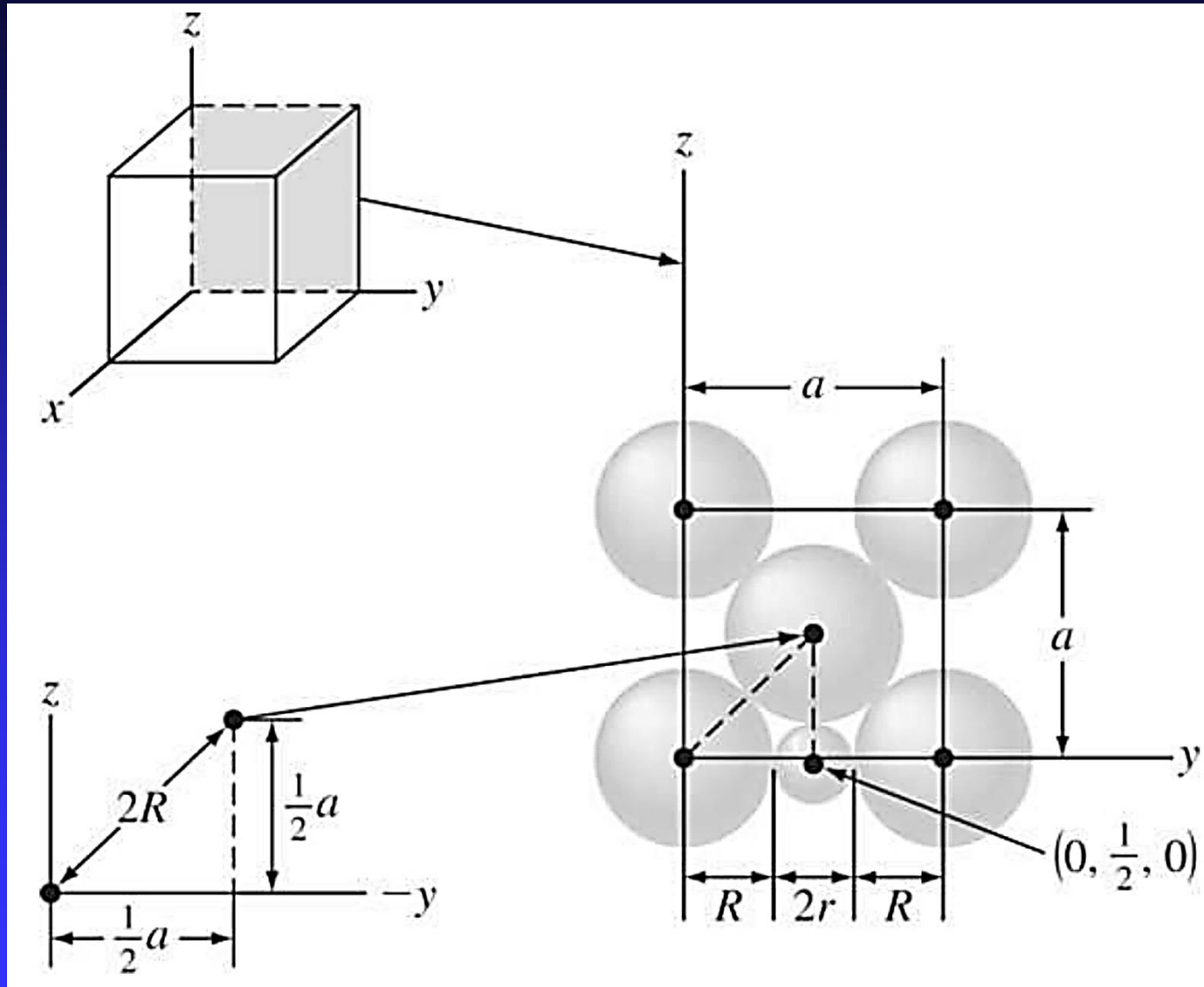
Aristas: $12 / 4 \text{ celdas} = 3 \text{ huecos / celda}$

Centro celda = 1 hueco / celda

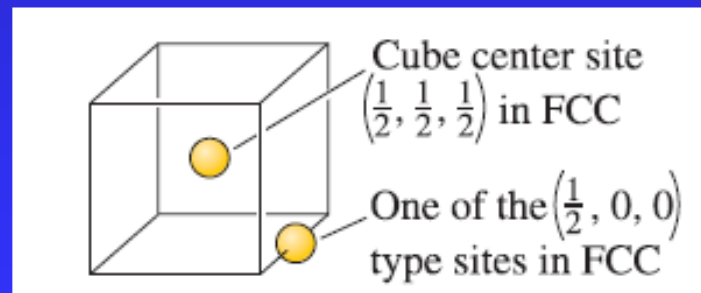
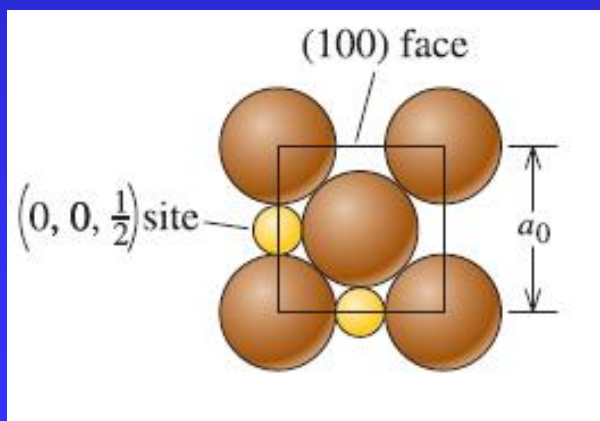
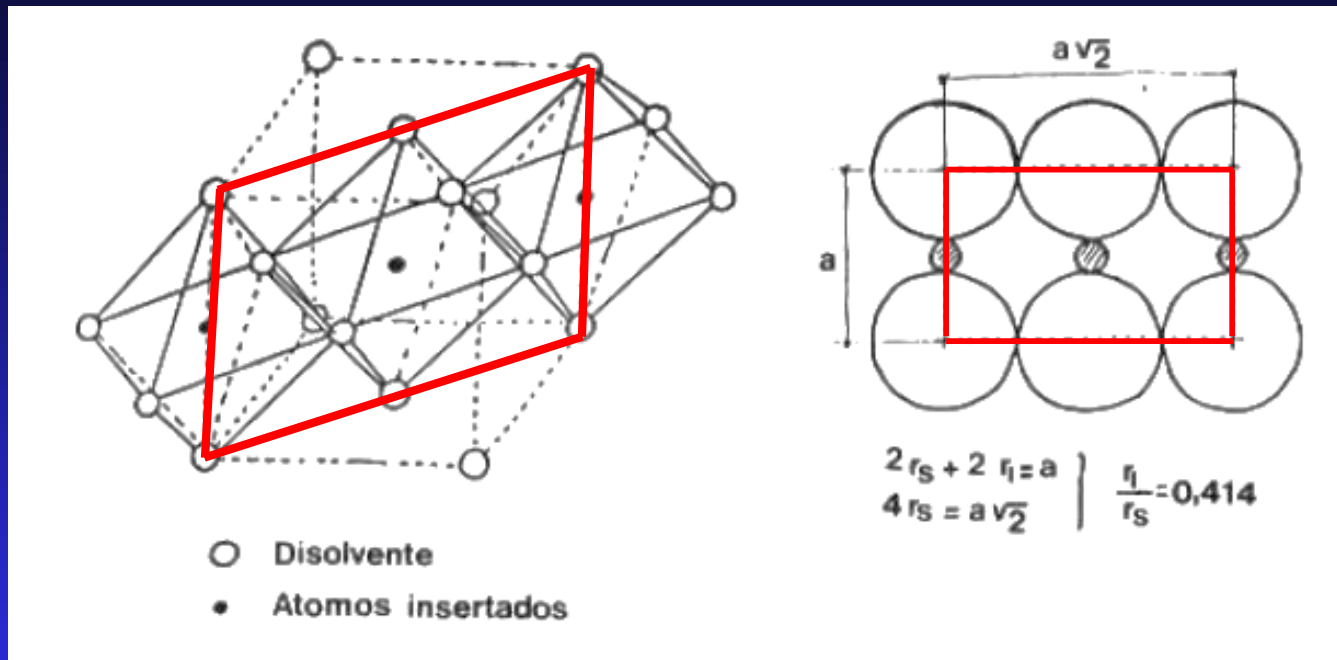
ATOMOS INSERTADOS = 4 átomos/celda



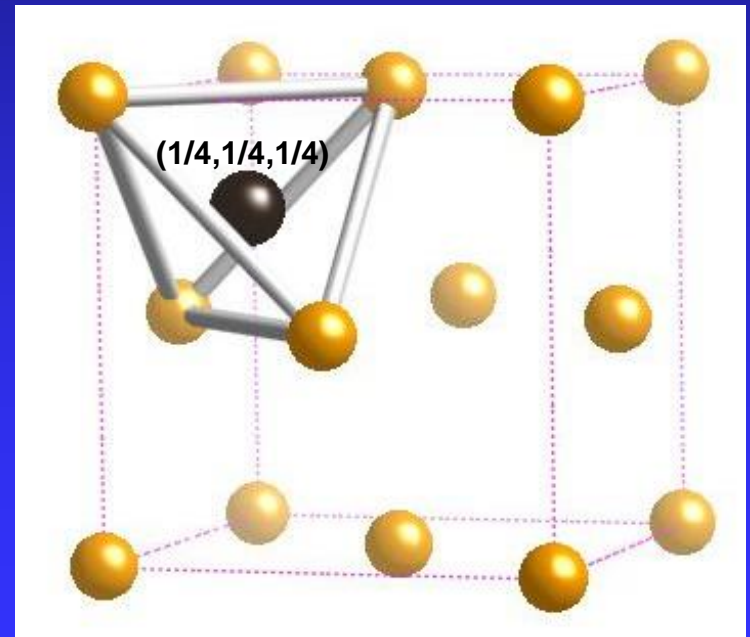
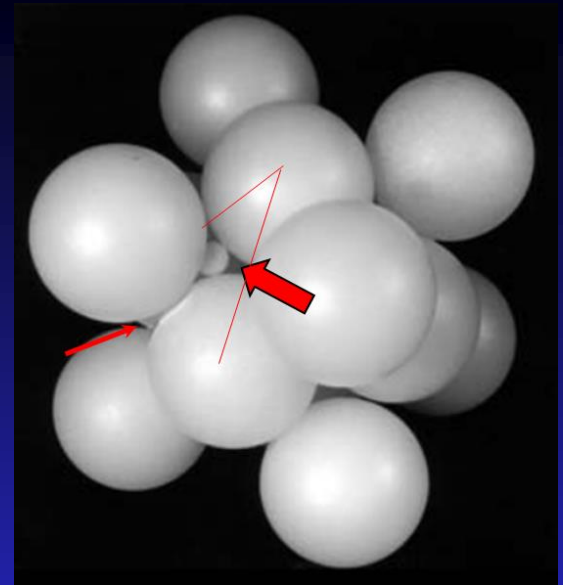
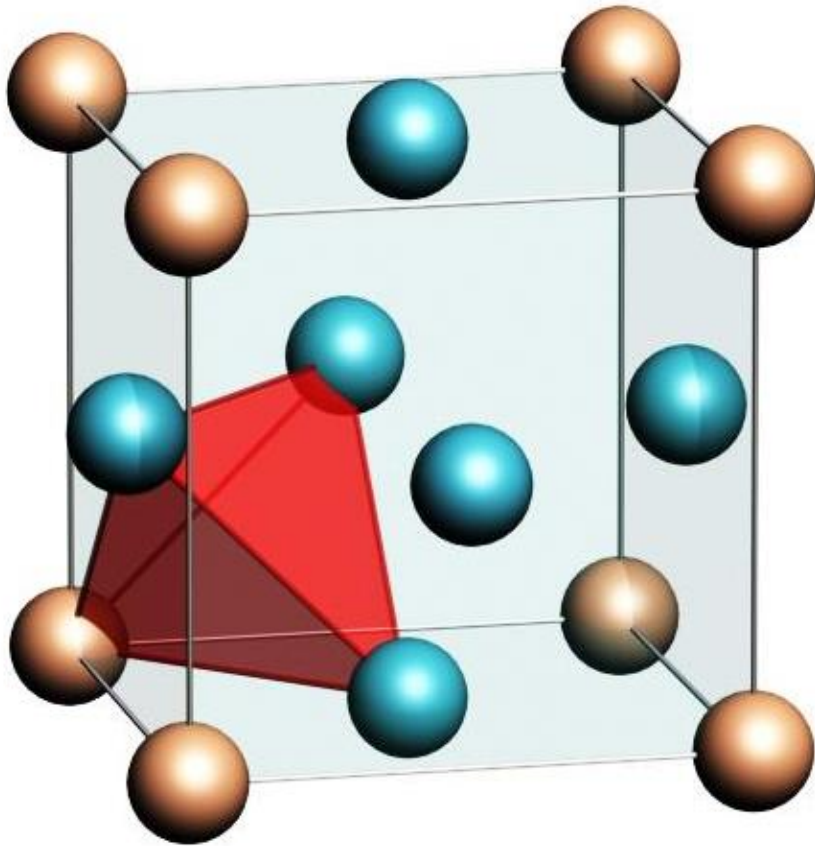
Sistema FCC: Inserción octaédrica



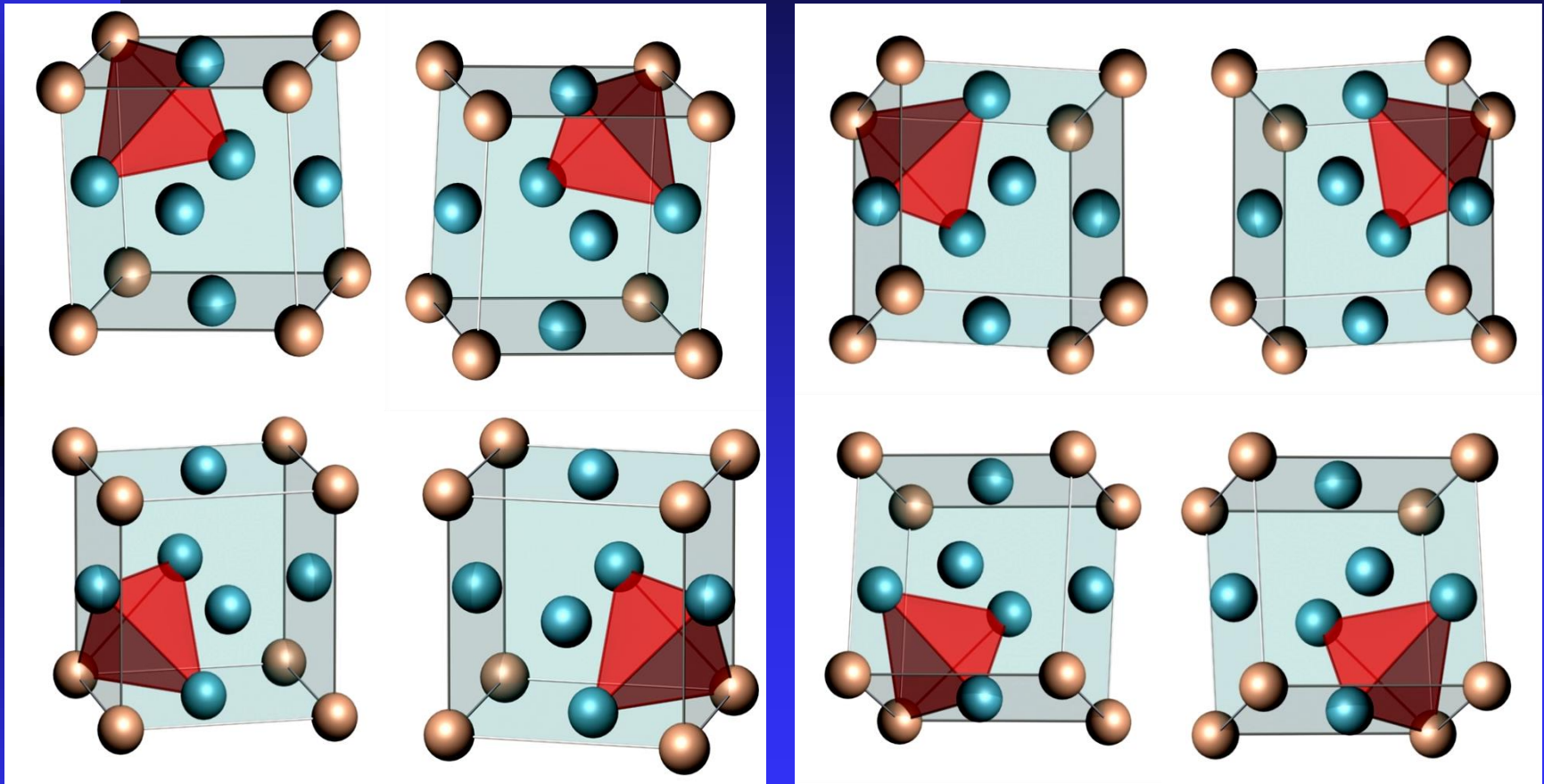
FCC. Huecos octaédricos: r_i/r_s



Sistema FCC: Huecos tetraédricos

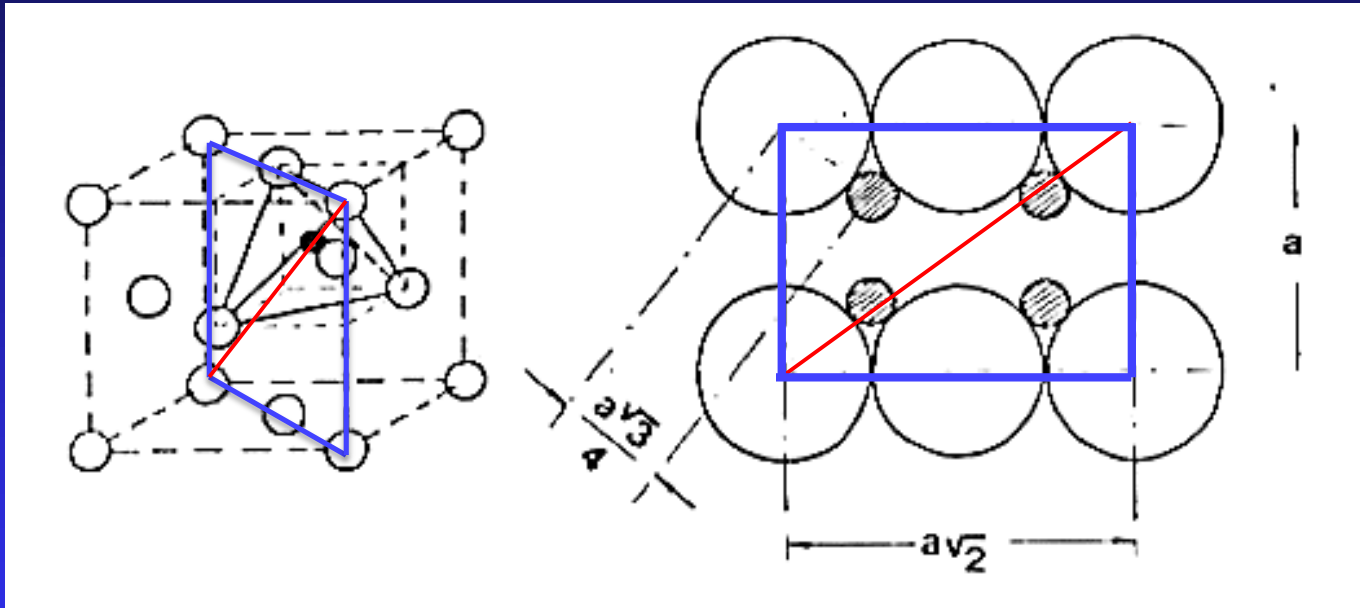


FCC: Huecos tetraédricos (8 huecos/celda)



Huecos internos, dentro de la celda

FCC. Huecos tetraédricos: r_i/r_s

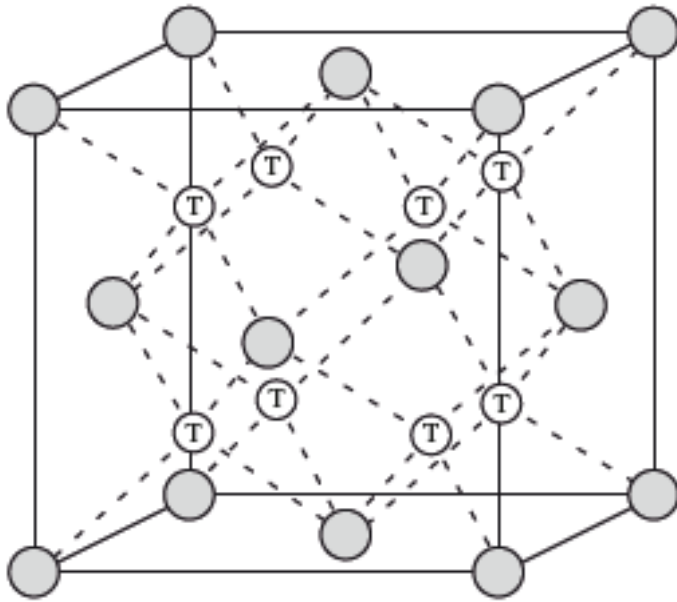


$$2 r_s = \frac{a \sqrt{2}}{2} \quad r_s + r_i = \frac{a \sqrt{3}}{4}$$

$$\frac{r_i}{r_s} = \frac{a \sqrt{3}/4}{a \sqrt{2}/4} - 1 = 0,225$$

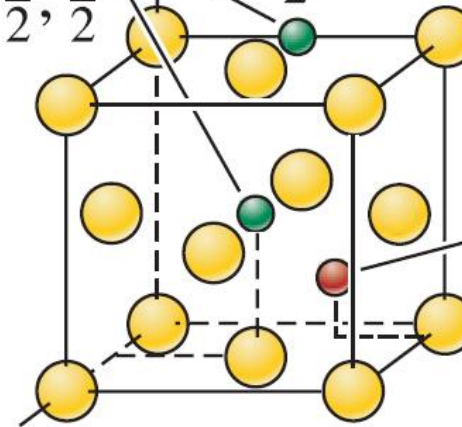
Sistema FCC: Inserciones tetraédricas y octaédricas

Huecos tetraédricos \Rightarrow 8 átomos/celda



Octahedral

$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ $0, \frac{1}{2}, 1$

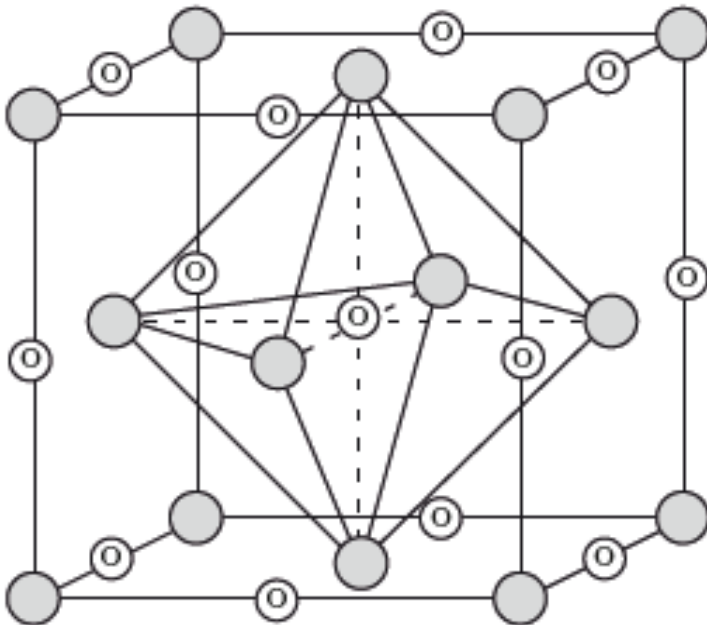


Tetrahedral

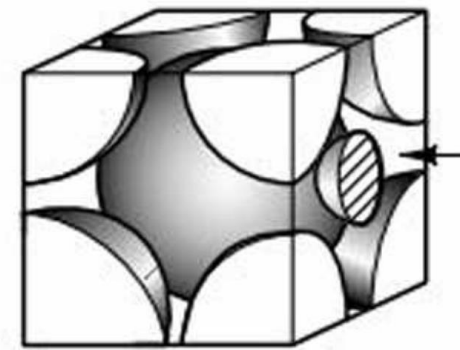
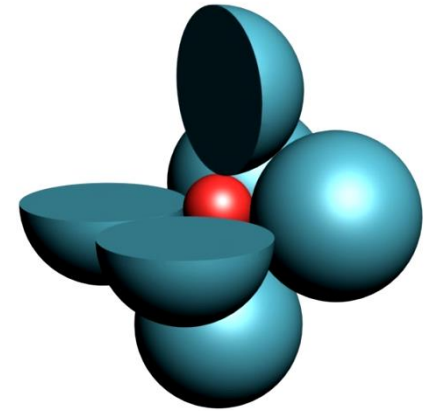
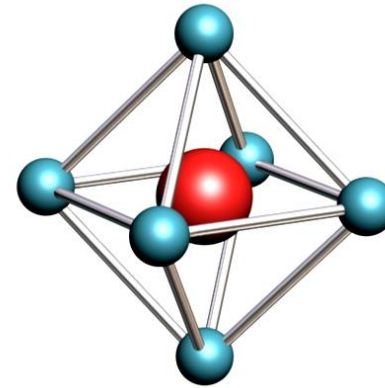
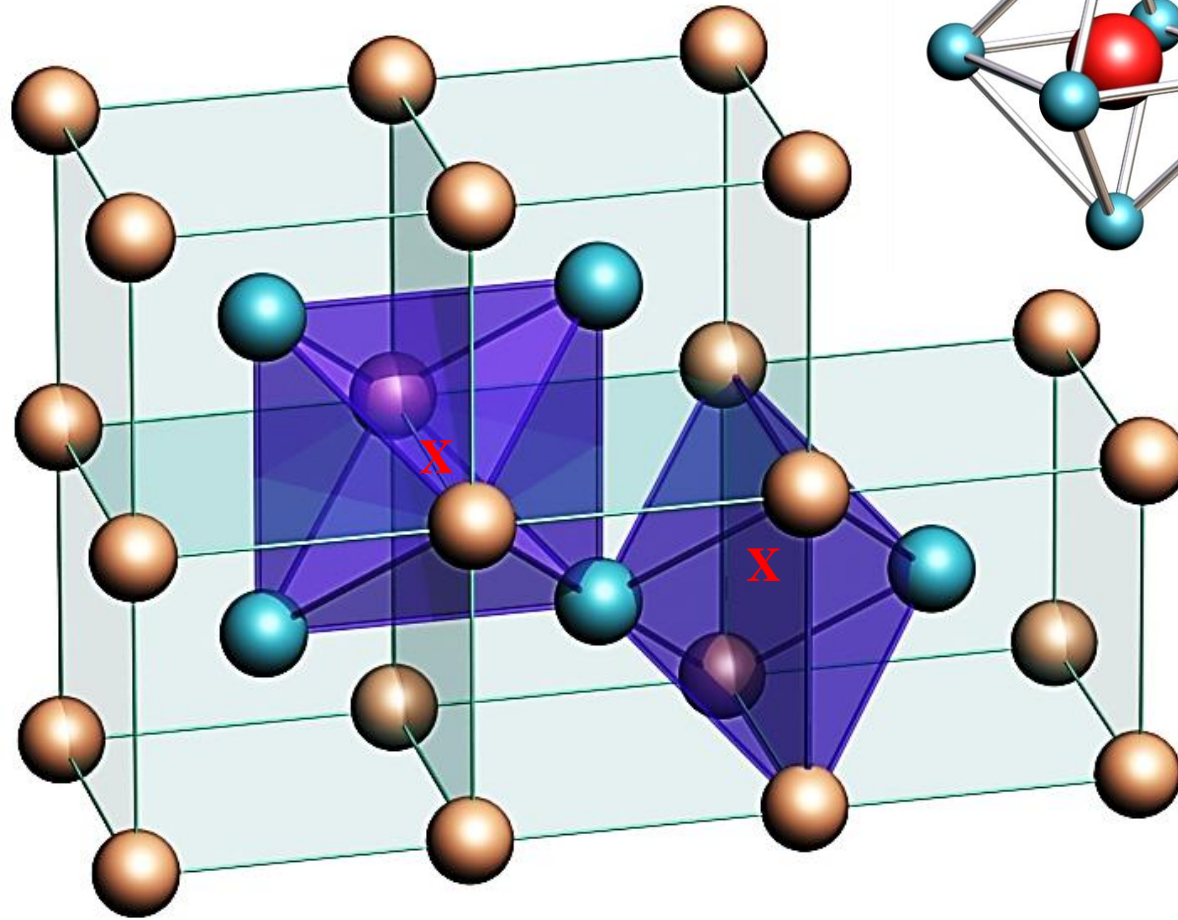
$\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$

FCC

Huecos octaédricos \Rightarrow 4 átomos/celda

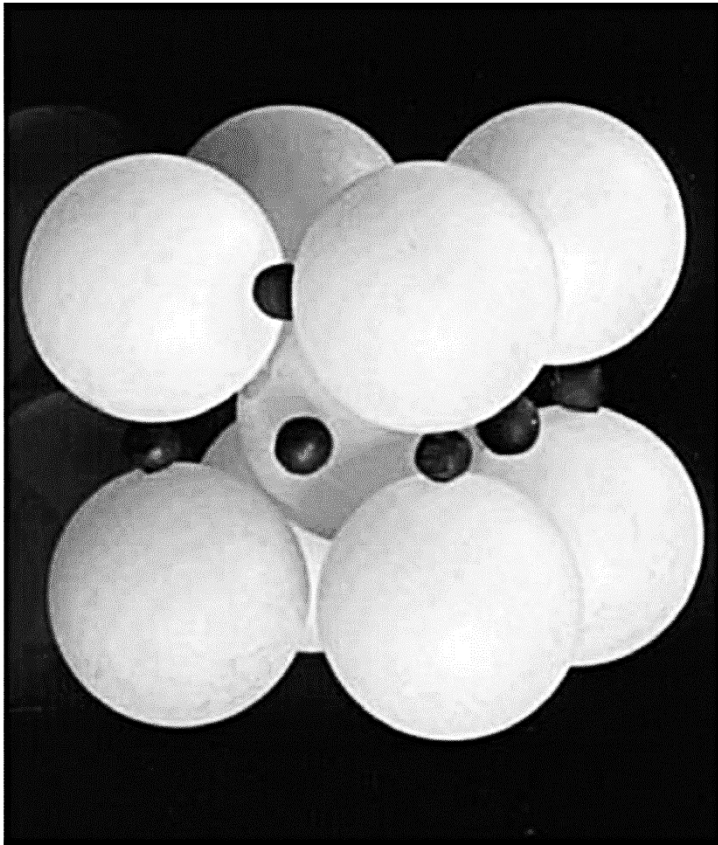


Sistema BCC: Huecos octaédricos

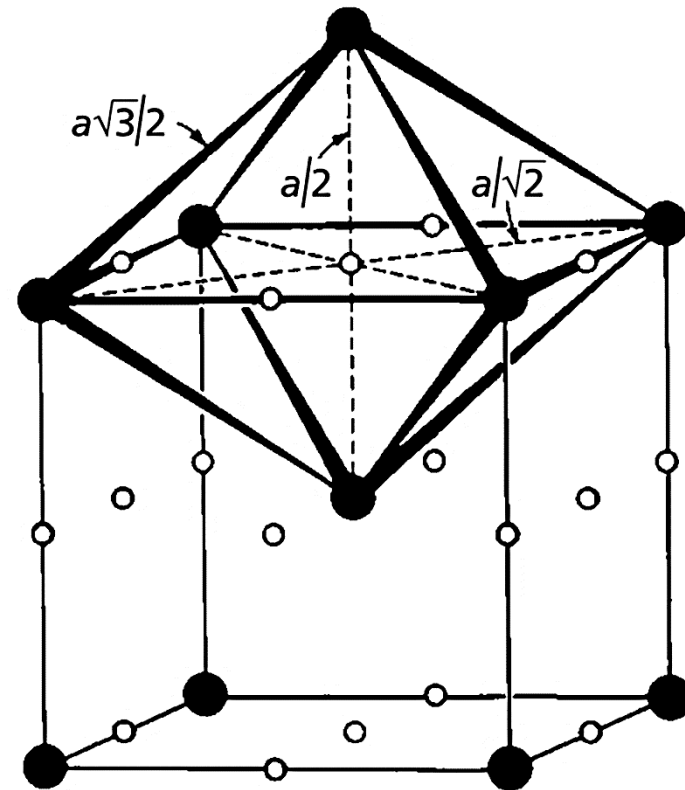


$$(12 \text{ aristas} / 4 \text{ celdas}) + (6 \text{ caras} / 2 \text{ celdas}) = 6 \text{ huecos} / \text{celda}$$

Sistema BCC: Huecos octaédricos



(a)

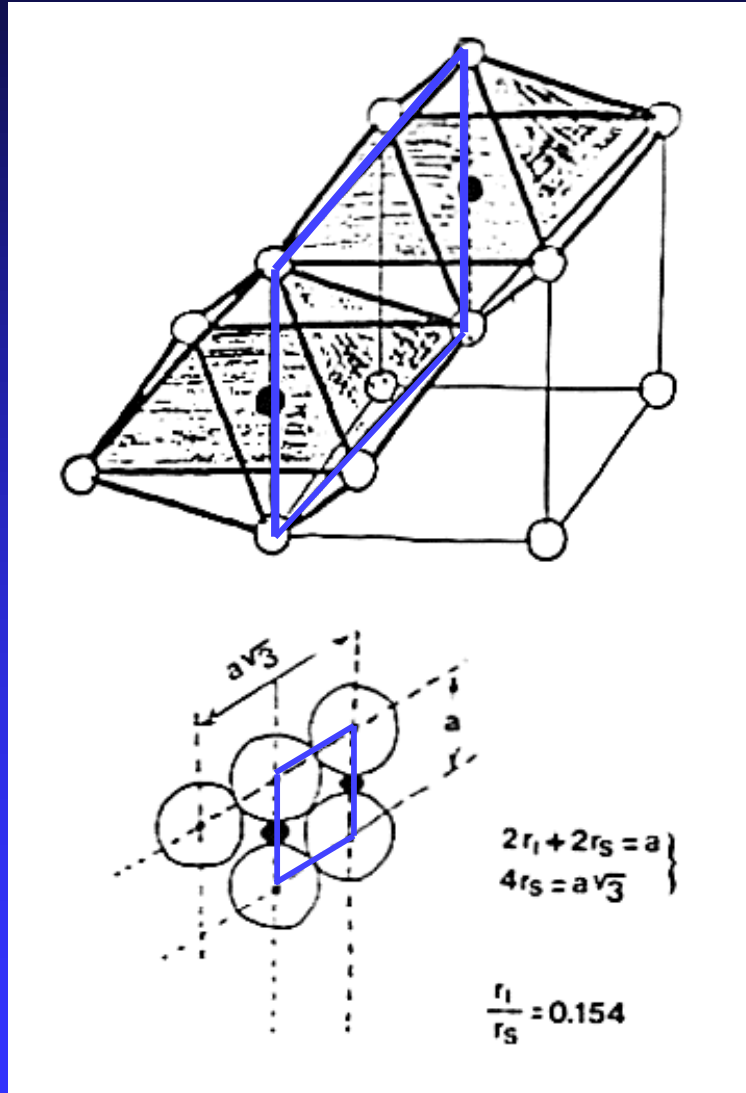


- Metal atoms
○ Octahedral interstices

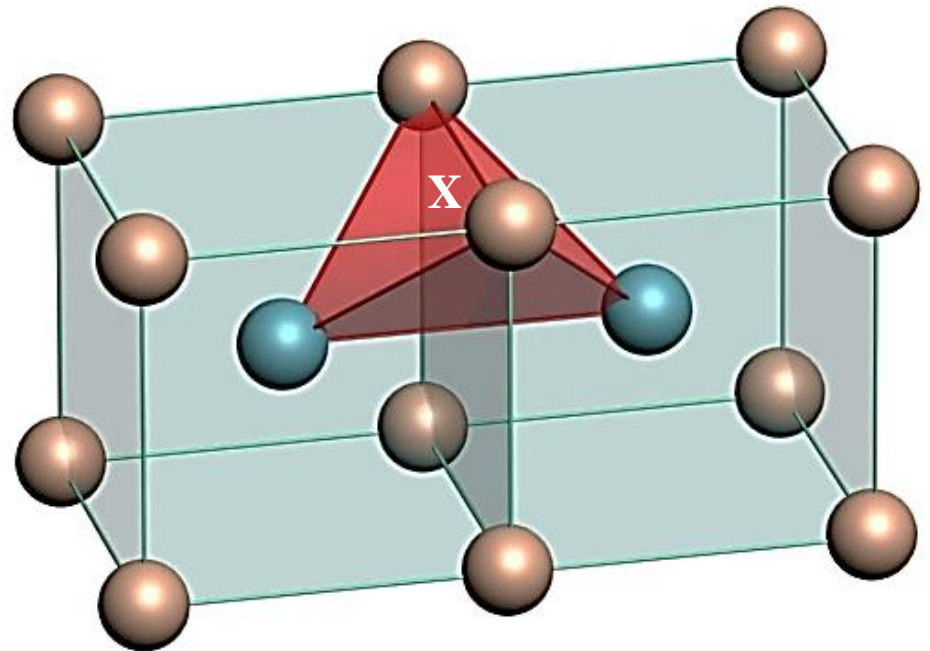
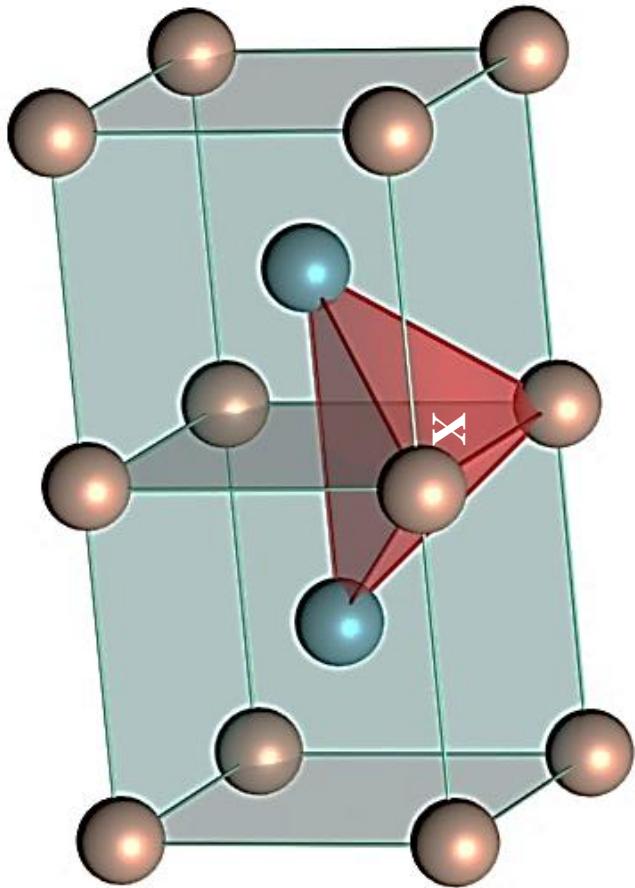
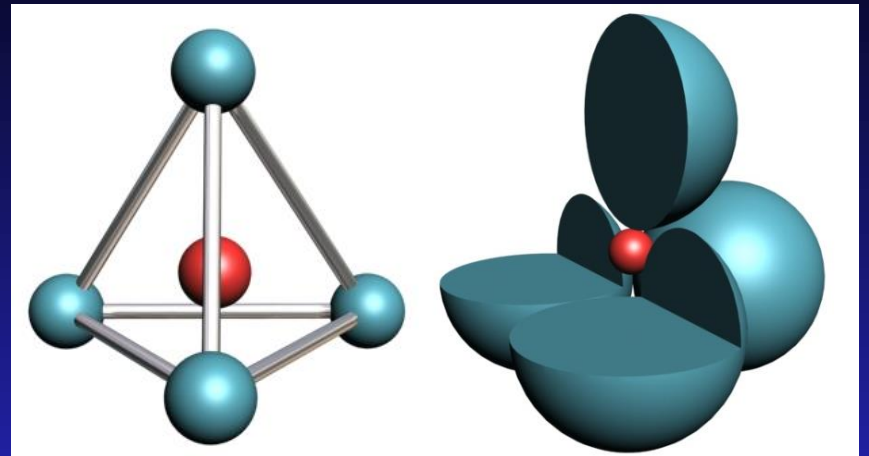
(b)

(6 huecos /caras / 2 celdas) \Rightarrow **3 átomos / celda**
(12 huecos /caras / 4 celdas) \Rightarrow **3 átomos / celda**
6 átomos/celda

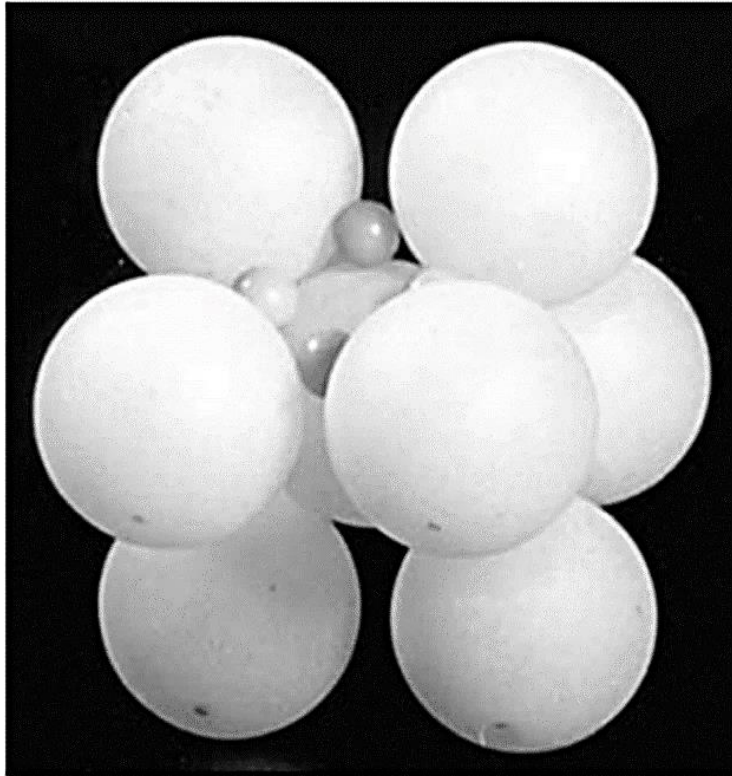
BCC. Huecos octaédricos: r_i/r_s



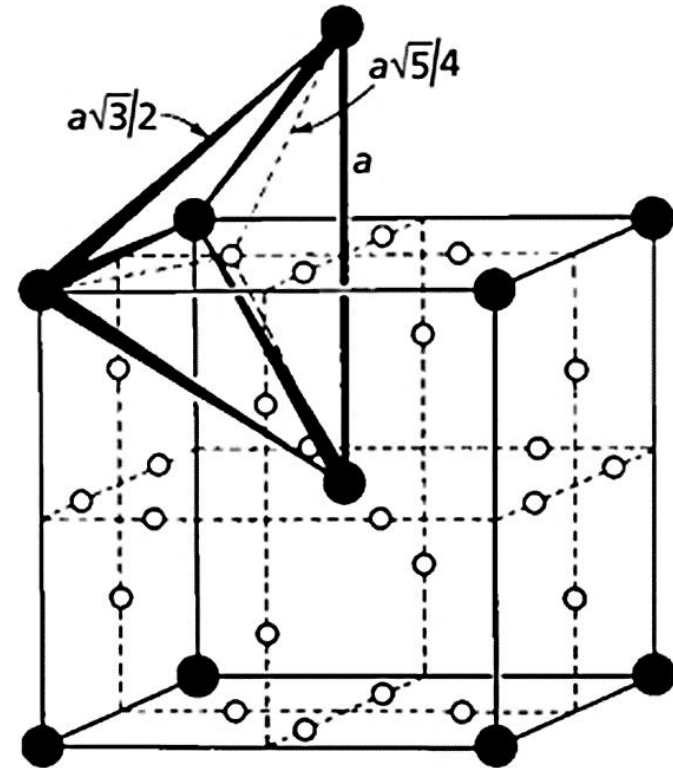
Sistema BCC: Huecos tetraédricos



Sistema BCC: Huecos tetraédricos



(c)

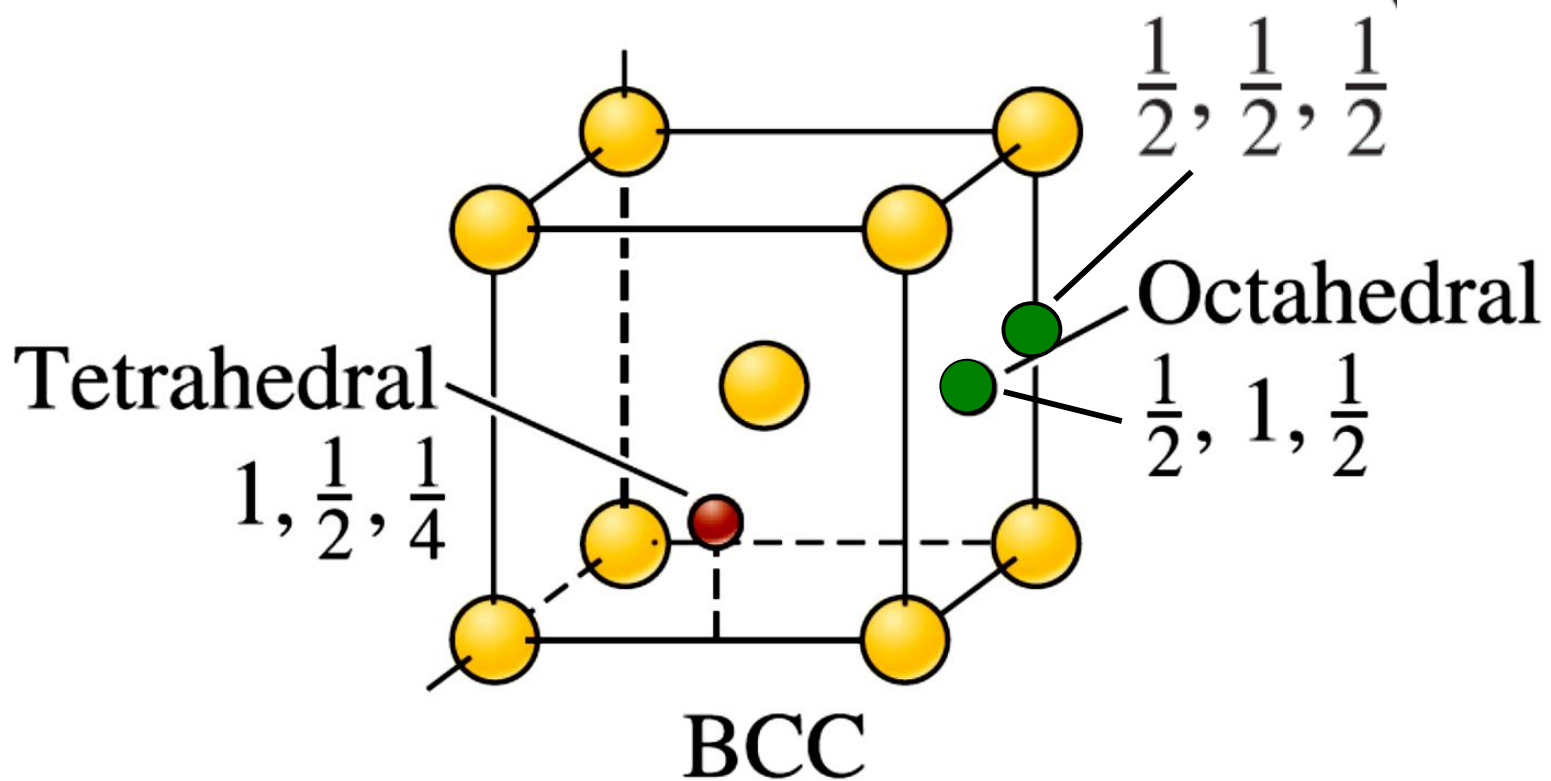


● Metal atoms

(d) ○ Tetrahedral interstices

6 caras (4 huecos / 2 celdas) \Rightarrow **12 átomos / celda**

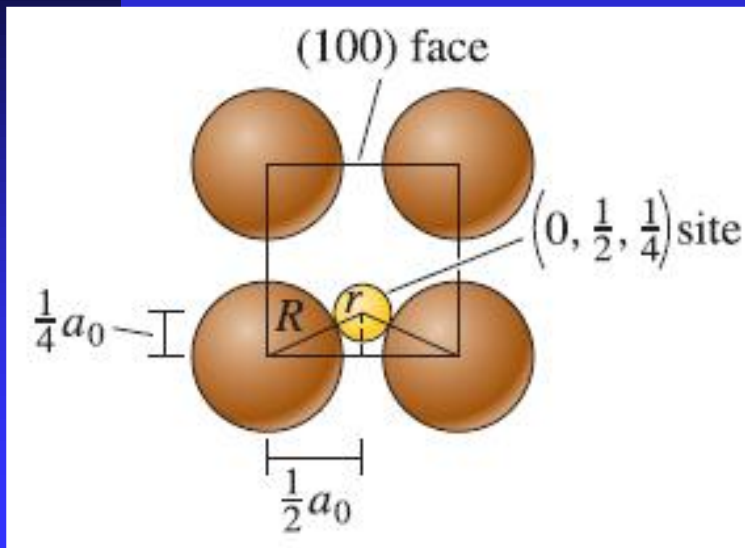
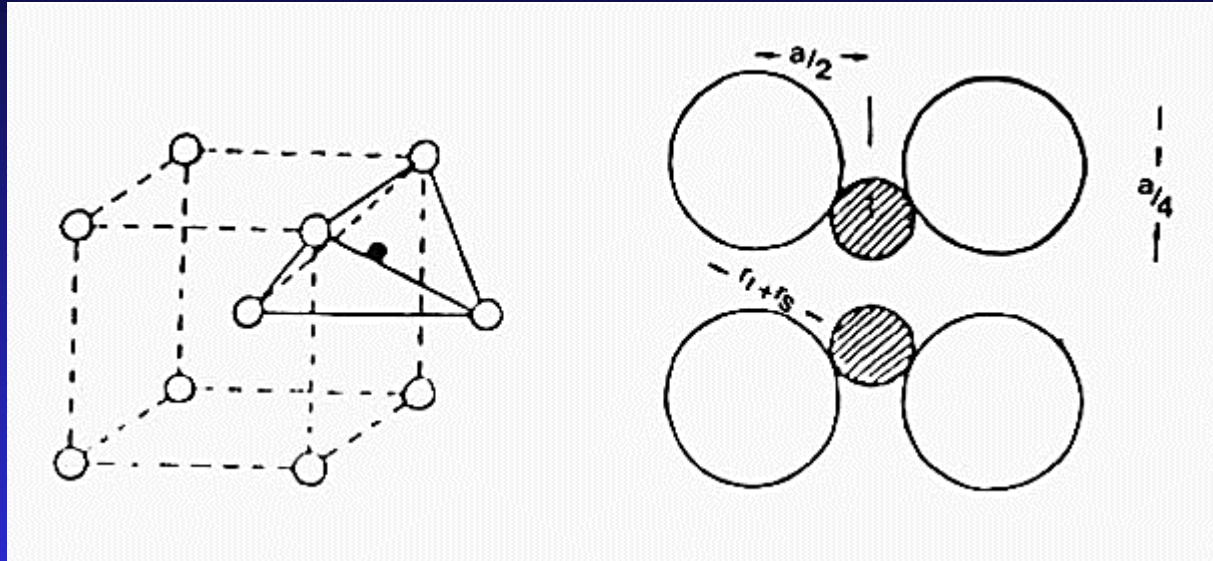
Sistema BCC: Inserciones tetraédricas y octaédricas



Huecos tetraédricos \Rightarrow **12 átomos**

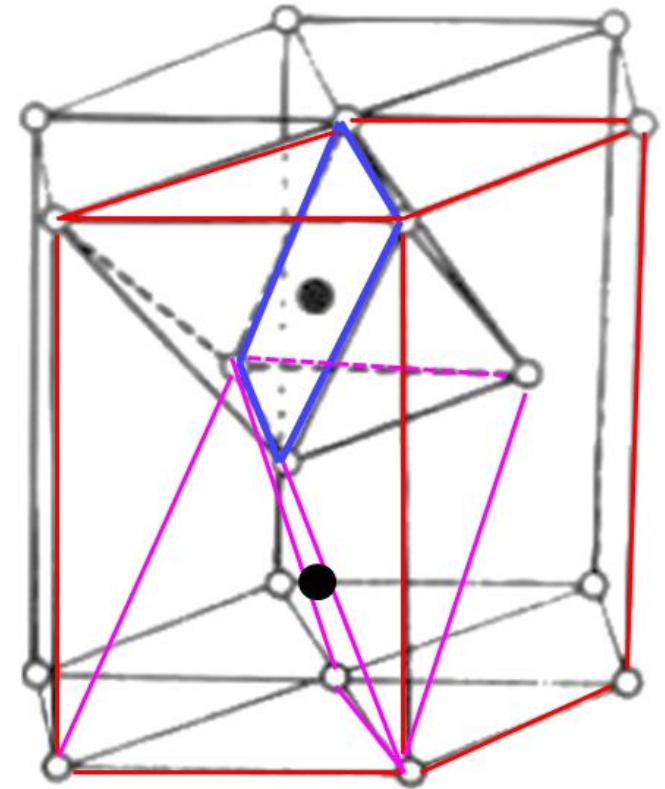
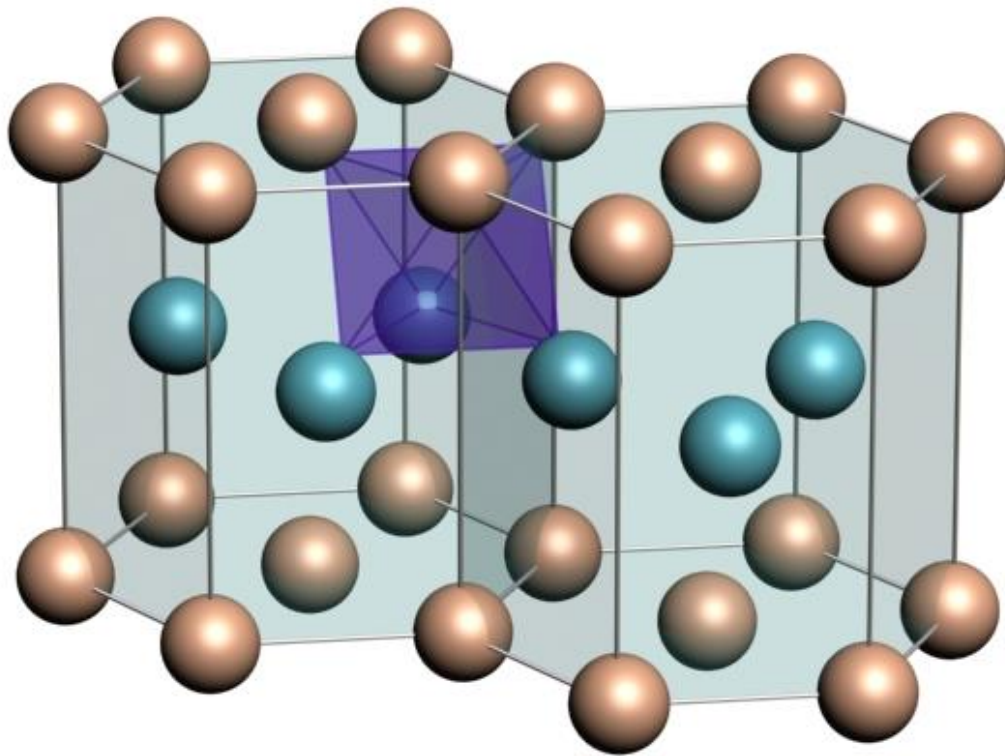
Huecos octaédricos \Rightarrow **6 átomos**

Sistema BCC: Huecos tetraédricos



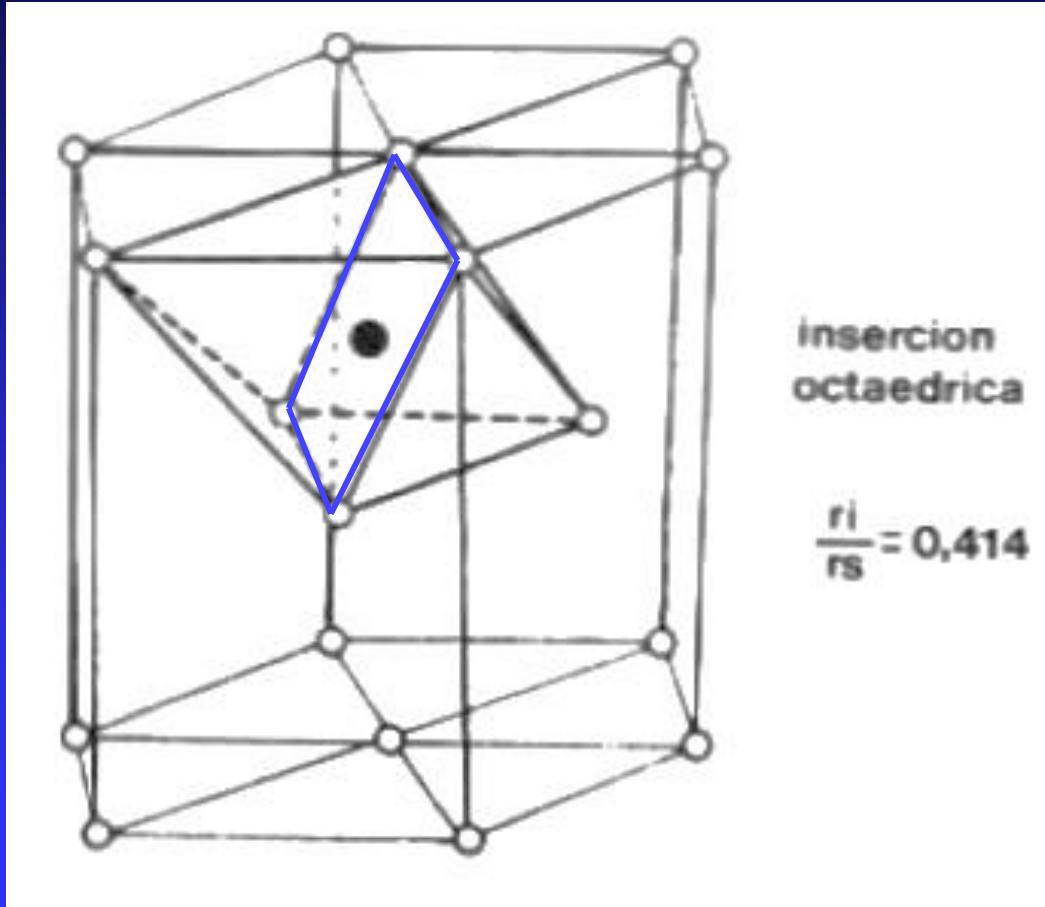
$$\left. \begin{aligned} (r_1 + r_s)^2 &= \frac{a^2}{4} + \frac{a^2}{16} \rightarrow r_1 + r_s = \frac{a\sqrt{5}}{4} \\ 4r_s &= a\sqrt{3} \end{aligned} \right\} r_1/r_s = 0.291$$

SISTEMA HC: Huecos octaédricos

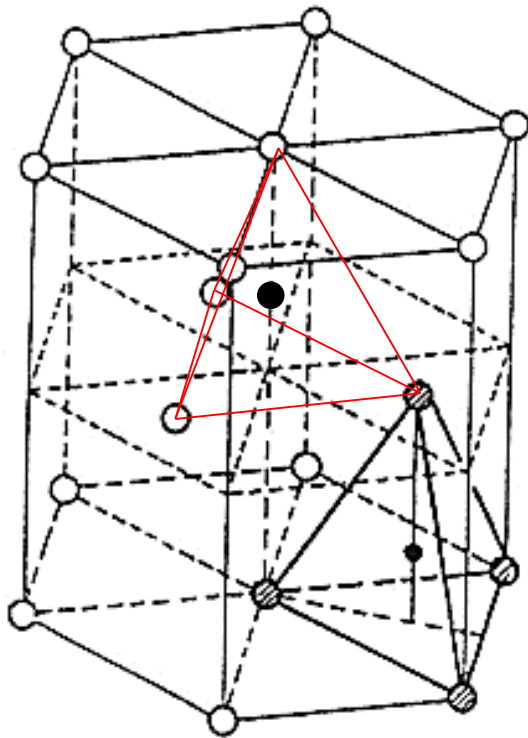


Intersticios octaédricos \Rightarrow **6 huecos/celda**

HC. Huecos octaédricos: r_i/r_s

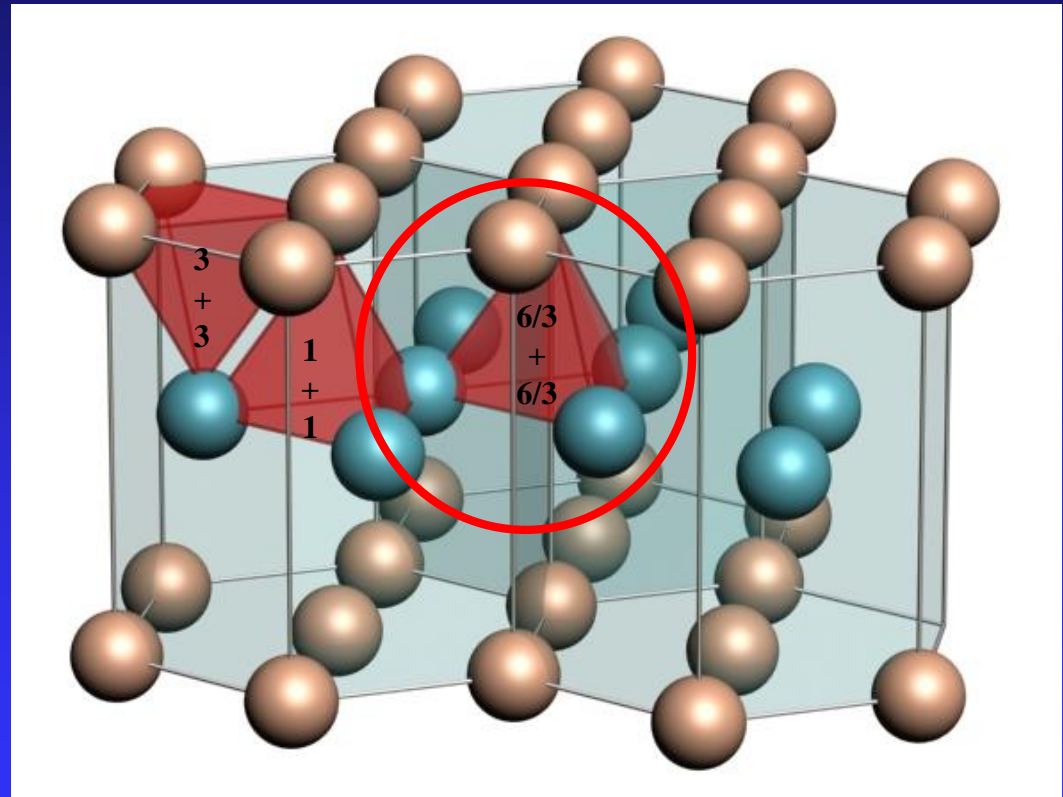


SISTEMA HC: Huecos tetraédricos



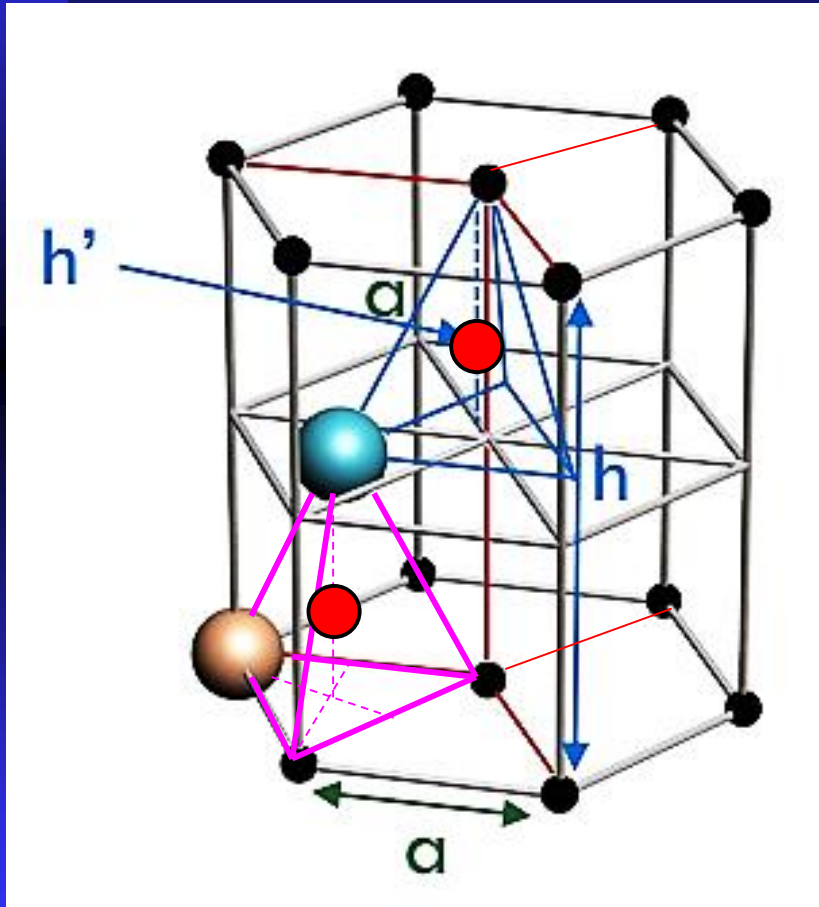
- Site interstitiel T
- Atome du métal H.C.

*Maille HC; site
interstitiel tétraédrique.*



Intersticios tetraédricos: 12 huecos/celda

SISTEMA HC: Huecos tetraédricos



- ❖ **6 huecos/celda** con tetraedros de las bases.
- ❖ **2 huecos/celda** con tetraedros centrales.
- ❖ **(12/3) huecos/celda** de las aristas
- ❖ **12 ATOMOS/CELDA**

HC. Huecos tetraédricos: r_i/r_s

