

Z. nb (atome) par maille

$$Z = A \times \frac{1}{8} + M \times \frac{1}{2} + N \times \frac{1}{4} + P \times 1$$

masse volumique: ρ

$$\rho = \frac{\text{masse (maille)}}{V_{\text{maille}}} = \frac{Z \times \text{masse (atome)}}{V_{\text{maille}}}$$

$$\rho = \frac{Z \cdot M_{\text{atome}}}{N_A \cdot V_{\text{maille}}}$$

Capacité: $\gamma < 1$

$$\gamma = \frac{V_{\text{occupie}}}{V_{\text{maille}}} = \frac{Z \cdot V_{\text{atome}}}{V_{\text{maille}}}$$

Alr: un cristal métallique des brs cubique (c)

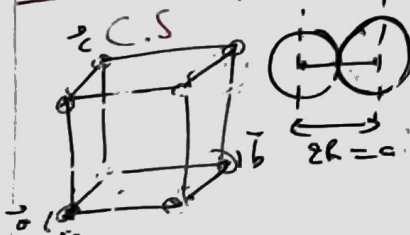
atome: atome

maille: Cubique (c)

$$\rho = \frac{Z \cdot M_{\text{atome}}}{N_A \cdot a^3}$$

$$\gamma = \frac{Z \times \frac{4}{3} \pi R^3}{a^3}$$

mode 2: Cubique simple



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

Coordonnées réduites (0,0,0)

Mode de Translation par translation

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

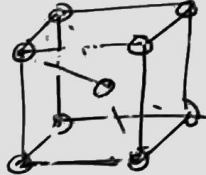
$$\rho = \frac{1 \times M_{\text{atome}}}{N_A \cdot a^3}; \gamma = \frac{1 \times \frac{4}{3} \pi R^3}{a^3}$$

$$a \cdot 2R = a$$

$$\gamma = \frac{\frac{4}{3} \pi R^3}{(2R)^3} = 0.58$$

Sys Cubique: 3 modes de Bravais

mode 1: Cubique centrée: C.C



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

$$Z = 1 + 1 = 2$$

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

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

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

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

$$\gamma = \frac{2 \times \frac{4}{3} \pi R^3}{a^3}$$

$$\gamma = \frac{2 \times \frac{4}{3} \pi R^3}{(\frac{4R}{\sqrt{3}})^3} = 0.68$$

mode F: Cubique à faces centrées: C.F.C



$$Z = 8 \times \frac{1}{8} + 6 \times \frac{1}{2} = 1 + 3$$

$$Z = 4$$

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

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

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

$$\gamma = \frac{4 \times \frac{4}{3} \pi R^3}{a^3}; a \cdot 2R = \frac{a\sqrt{2}}{2}$$

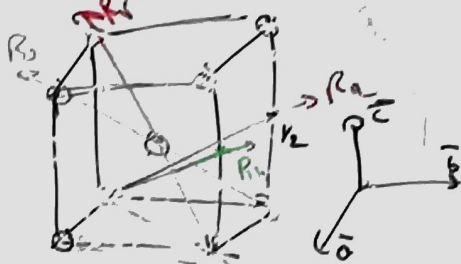
$$\gamma = \frac{4 \times \frac{4}{3} \pi R^3}{(\frac{a\sqrt{2}}{2})^3} = 0.74$$

Rangee Cristalline: $R[uvw]$

$$\vec{R} = \vec{ON} = u\vec{a} + v\vec{b} + w\vec{c}$$

u, v, w : entiers premiers entre eux

$$\Rightarrow \Pi(u, v, w)$$



$$\vec{R}_1 = \vec{a} + \vec{b} + 0\vec{c}$$

$$R_2[110]$$

$$R_3[\bar{1}\bar{1}1]$$

$$\vec{R}_3 = -\vec{a} - \vec{b} + \vec{c}$$

$$\vec{R}_2 = 0\vec{a} + \vec{b} + \frac{2}{2}\vec{c}$$

$$\vec{R}_2 = 0\vec{a} + 2\vec{b} + \vec{c}$$

$$R_2[021]$$

$$\vec{R}_3 = \vec{a} - \vec{b} + \vec{c}$$

$$R_3[1\bar{1}1]$$

$$R_4[221]$$

$$\vec{R}_u = 2\vec{a} + 2\vec{b} + \vec{c}$$

$$= 2(-\vec{a} + \vec{b} + \frac{1}{2}\vec{c})$$

famille de plans réticulaires (hkl)

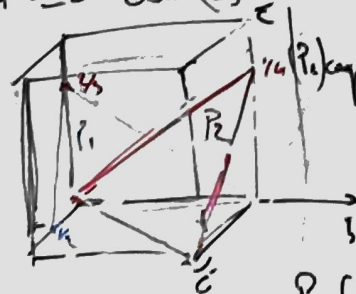
h, k, l : entiers

le plan de la famille (hkl) ne passe pas par l'origine O.

$$\Leftrightarrow h=0 \text{ la } (P) \parallel \vec{OA}$$

$$\Leftrightarrow k=0 \text{ la } (P) \parallel \vec{OB}$$

$$\Leftrightarrow l=0 \text{ la } (P) \parallel \vec{OC}$$



$$(0x): A \mid \vec{OA} = \frac{\vec{a}}{h}$$

$$(0y): B \mid \vec{OB} = \frac{\vec{b}}{k}$$

$$(0z): C \mid \vec{OC} = \frac{\vec{c}}{l}$$

$$(0x): \vec{a} \cdot \frac{1}{h}$$

$$(0y): \vec{b} \cdot \frac{1}{k}$$

$$(0z): \vec{c} \cdot \frac{1}{l}$$

$$P_2(423)$$

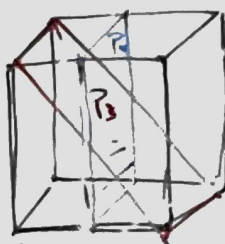
parallèle
équidistant: $d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$

le plan de la famille (hkl) coupe

$$(0x): A' \mid \vec{OA'} = n \cdot \frac{\vec{a}}{h}$$

$$(0y): B' \mid \vec{OB'} = n \cdot \frac{\vec{b}}{k}$$

$$(0z): C' \mid \vec{OC'} = n \cdot \frac{\vec{c}}{l}$$



$$P_3 \parallel \vec{a}(0x): h=0$$

$$\Rightarrow P_3(011)$$

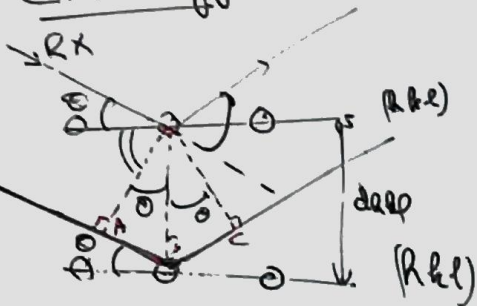
$$P_2 \text{ coupe } \begin{cases} (0x): \vec{a} \cdot \frac{1}{h} \\ (0y): \vec{b} \cdot \frac{1}{k} \\ (0z): \vec{c} \cdot \frac{1}{l} \end{cases}$$

$$P_2(3\bar{3}4)$$

$$P_4(020)$$

Diffraction aux RX
 $\lambda \in [a, 2,1 \text{ \AA}]$

Loi de Bragg



$$\delta = AB + BC$$

$$\sin \theta = \frac{AB}{d \sin \theta} = \frac{BC}{d \sin \theta}$$

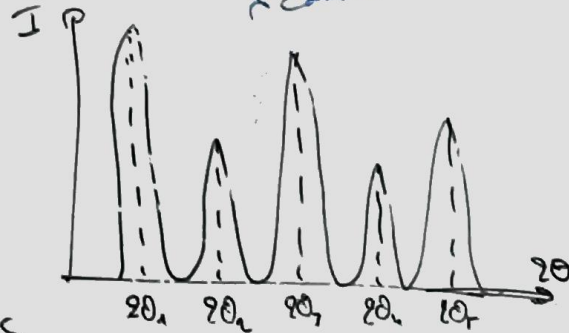
$$\delta = 2d \sin \theta = m\lambda$$

$$AB = BC = d \sin \theta$$

m. ordre de diffraction

m = 1 : diffraction du 1^{er} ordre

différence de marche optique
 $\delta = m\lambda$
 λ connue.



Conditions de diffraction

mode I : tous les plans (hkl) diffractent (221)
 (hkl) (100) (110) (111) (200) (210) (211) (220) (300)

$$(h^2 + k^2 + l^2): 1 \quad 2 \quad 3 \quad 4 \quad 5 \quad 6 \quad 8 \quad 9$$

mode I : les plans (hkl) diffractent / (h+k+l) = 2n

$$(hkl) \quad (110) \quad (200) \quad (211) \quad (220) \quad (310) \quad (222)$$

$$h^2 + k^2 + l^2 \quad 2 \quad 4 \quad 6 \quad 8 \quad 10 \quad 12$$

mode F : les plans (hkl) qui diffractent / h, k, l sont pairs

$$(hkl): (111); (200); (220); (311); (222)$$

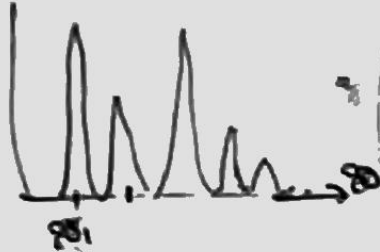
$$(h^2 + k^2 + l^2): 3 \quad 4 \quad 8 \quad 11 \quad 12$$

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

$$(h^2 + k^2 + l^2) = \left(\frac{a}{d_{hkl}}\right)^2$$

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

Diffraction aux RX
 $\lambda \in [\text{ar}, 2.1 \text{ \AA}]$



$\epsilon^{\text{con}} : (a)_{\text{inconnue}}$

mode I : la 1^{ère} réflexion (100)

$$d_1 = a$$

$$d_{\text{all}} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

$$\left(\frac{d_1}{d_{\text{all}}}\right)^2 = (h^2 + k^2 + l^2)$$

mode I : la 1^{ère} réflexion (100)

$$d_2 = \frac{a}{\sqrt{2}} \quad \left\{ 2 \left(\frac{d_1}{d_{\text{all}}}\right)^2 = h^2 + k^2 + l^2 \right.$$

mode F : la 1^{ère} réflexion (111)

$$d_1 = \frac{a}{\sqrt{3}} \quad \left\{ 3 \left(\frac{d_1}{d_{\text{all}}}\right)^2 = h^2 + k^2 + l^2 \right.$$

1^{ère} con : a connue : $d_{\text{all}} = \frac{a}{2 \sin \theta_i}$

θ_i	$d_{\text{all}} = d_i$	mode I	mode F
θ_1	$\left(\frac{a}{d_1}\right)^2 : 1$	$\left(\frac{a}{d_1}\right)^2 : 2$	$\left(\frac{a}{d_1}\right)^2 : 3 (111)$
θ_2	$\left(\frac{a}{d_2}\right)^2 : 2$	$\left(\frac{a}{d_2}\right)^2 : 4$	$\left(\frac{a}{d_2}\right)^2 : 4 (200)$
θ_3	$\left(\frac{a}{d_3}\right)^2 : 3$	$\left(\frac{a}{d_3}\right)^2 : 6$	$\left(\frac{a}{d_3}\right)^2 : 8 (220)$
θ_4	$\left(\frac{a}{d_4}\right)^2 : 4$	$\left(\frac{a}{d_4}\right)^2 : 8$	$\left(\frac{a}{d_4}\right)^2 : 11 (211)$
θ_r	$\left(\frac{a}{d_r}\right)^2 : r$	$\left(\frac{a}{d_r}\right)^2 : 10$	$\left(\frac{a}{d_r}\right)^2 : 12 (222)$

$n = n$

$$(b^2, b^2 + p^2)$$

			mod I: $\left(\frac{d_i}{d_i}\right)^2$	mod I: $2\left(\frac{d_i}{d_i}\right)^2$	mod F: $3\left(\frac{d_i}{d_i}\right)^2$	
θ_i	$d_{11} = d_i$	$\left(\frac{d_i}{d_i}\right)^2$	1	2	3	3 (111)
θ_1	d_1	$\left(\frac{d_1}{d_1}\right)^2$	1	2	3	3 (111)
θ_2	d_2	$\left(\frac{d_1}{d_2}\right)^2$	2	4	4	4 (201)
θ_3	d_3	$\left(\frac{d_1}{d_3}\right)^2$	3	6	8	8 (220)
θ_4	d_4	$\left(\frac{d_1}{d_4}\right)^2$	4	8	11	11 (311)
θ_r	d_r	$\left(\frac{d_1}{d_r}\right)^2$	7	10	19	19 (242)
			mod F			

$$\theta_{\text{total}} = \frac{a}{\sqrt{b^2 + b^2 + p^2}}$$

$$a_1, a_2, a_3, a_4, a_r$$

$$\Rightarrow a = \frac{a_1 + a_2 + a_3 + a_4 + a_r}{r}$$