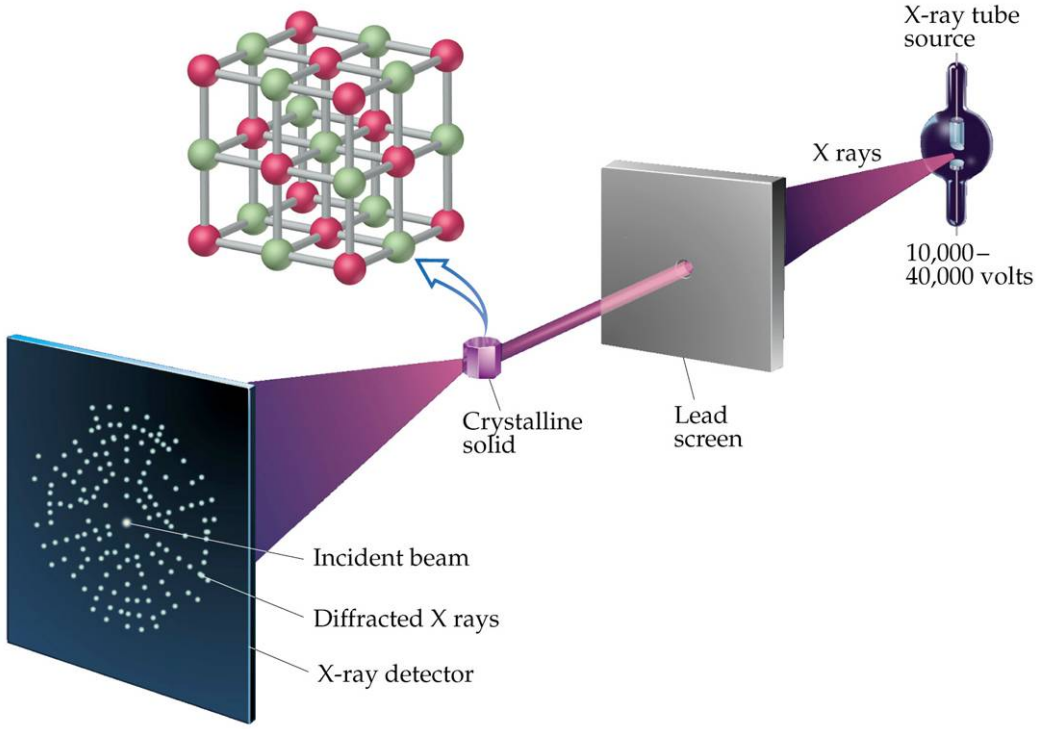
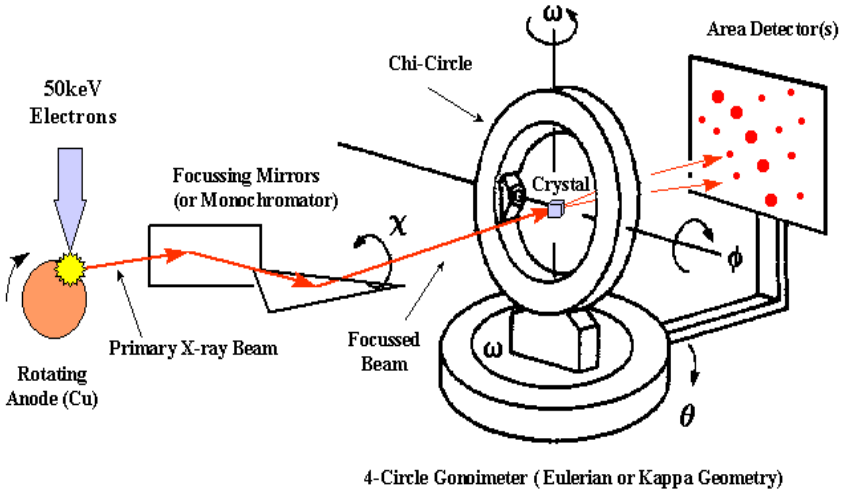
La diffraction des rayons X

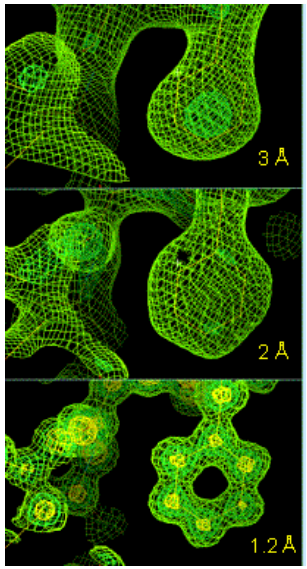
où comment retouver la position de 10^{23} atomes à partir d'un petit nombre de paramètres?

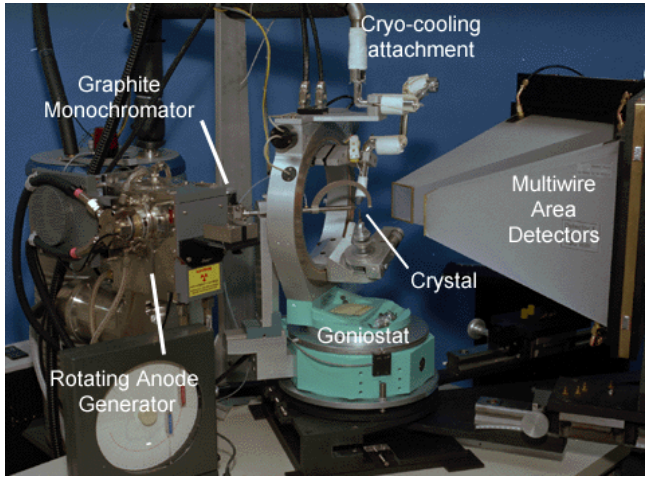


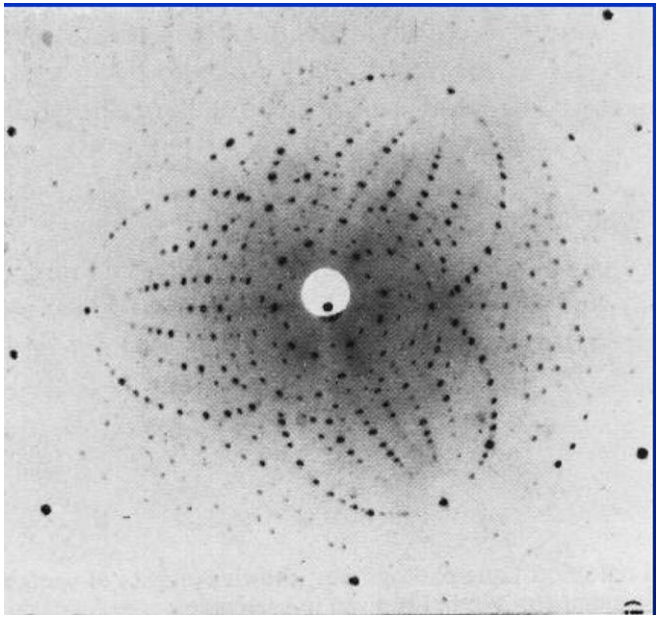
Structure des protéines

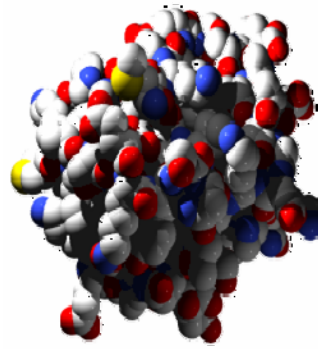


4-Circle Goniometer (Eulerian or Kappa Geometry)

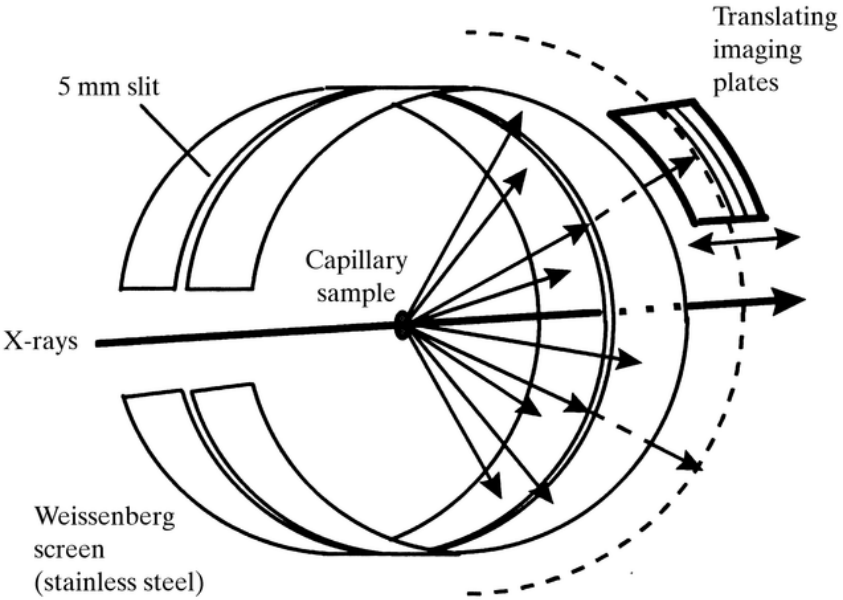




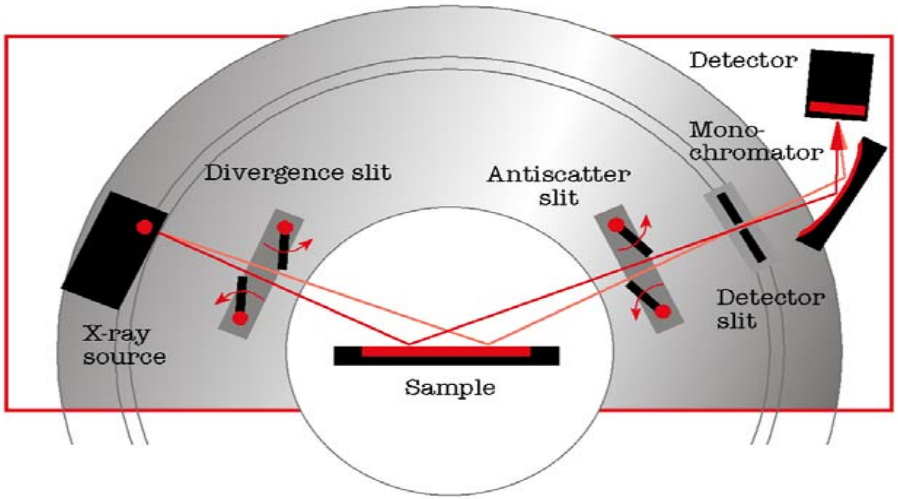


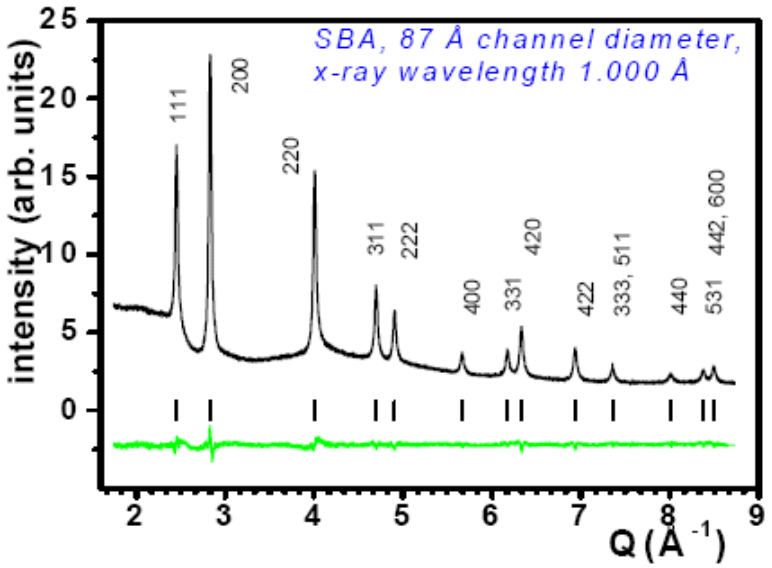


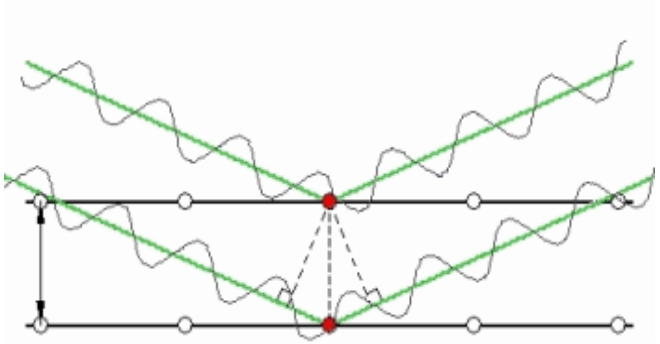
Debye Scherrer



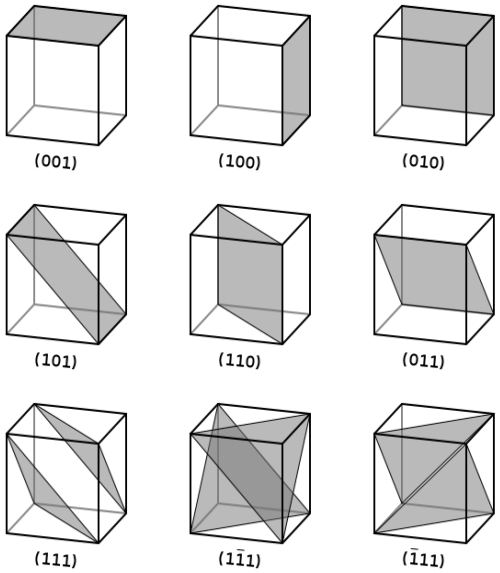
Bragg-Brentano







$$2d_{(hkl)}\sin\theta = n\lambda$$



$$I_{hkl} \propto m\,L(\theta).P(\theta).\left|F_{hkl}\right|^2$$

m : multiplicité = nb de plans équivalents

Table 3.3. Plane Multiplicity Factors, M_{hkl}

System	*hkl*	*hhl*	*hh*0	0*kk*	*hhh*	*hk*0	*h*0*l*	0*kl*	*h*00	0*k*0	00*l*
Cubic	48[a]	24	12	(12)	8	24[a]	(24[a])	(24[a])	6	(6)	(6)
Tetragonal	16[a]	8	4	(8)	(8)	8[a]	8	(8)	4	(4)	2
Hexagonal	24[a]	12[a]	6	(12)	(12)	12[a]	(12[a])	12[a]	6	(6)	2
Orthorhombic	8	(8)	(8)	(8)	(8)	4	(4)	(4)	2	(2)	(2)
Monoclinic	4	(4)	(4)	(4)	(4)	(4)	(2)	(4)	2	(2)	(2)
Triclinic	2	(2)	(2)	(2)	(2)	(2)	(2)	(2)	(2)	(2)	(2)

[a]When all permutations of indices do not produce equivalent planes, M must be reduced by half.

P facteur de polarisation (diffusion thomson) - pour une onde non polarisée

$$P(\theta) = \frac{1+\left(\cos(2\theta)\right)^2}{2}$$

L facteur de Lorentz (dépend de la géométrie de l'expérience : intersection entre la sphere d'Ewald et le réseau réciproque)

$$L(\theta) = \frac{1}{\sin^2(\theta)\cos(\theta)}$$

$\left|F_{hkl}\right|$ facteur de structure

$$\mathrm{F_{hkl}} = \sum_{\mathrm{j}} \mathrm{f_i}\, \mathrm{e}^{2\mathrm{i}\pi(\mathrm{hx_j}+\mathrm{ky_j}+\mathrm{lz_j})}$$

coefficient de diffusion atomique

Where B, the Debye-Waller temperature factor is:

$$f = f_0 \exp\left[-\frac{B\sin^2\theta}{\lambda^2}\right]$$

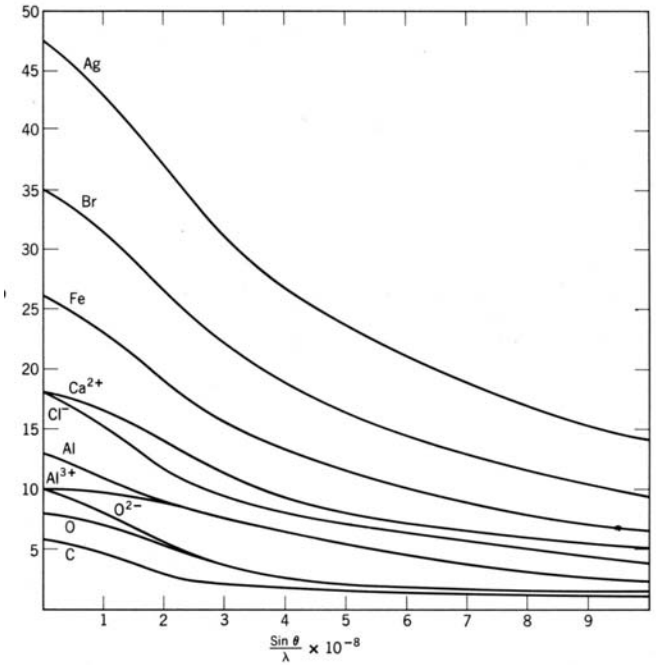


Fig. 3-15. Diffracting power of a few common atoms and ions (after C. W. Bunn, *Chemical Crystallography*, Oxford University Press, 1945).

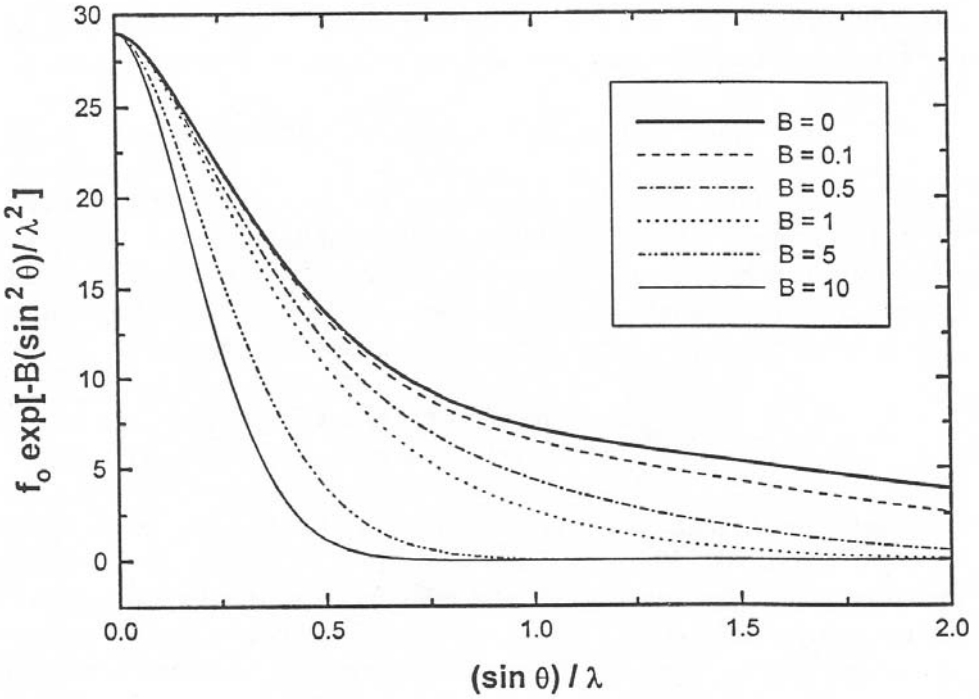
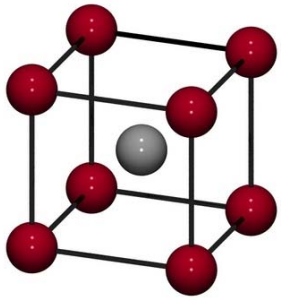


Figure 3.14. The effect of atomic thermal motion on the copper scattering factor.



Extinctions systématiques

$$F_{hkl} = \sum_j f_i e^{2i\pi(hx_j+ky_j+lz_j)}$$

For example, for a body-centered cubic cell, for each atom located at x, y, z there will be an identical atom located at x+½, y+½, z+½. The structure factor $\mathbf{F}_{hkl}$ is represented by the following equation.

$$\mathbf{F}_{hkl} = \left(\sum_{j=1}^{m/2} f_n \exp\left[2\pi i(hx_j + ky_j + lz_j\right] \right) + \left(\sum_{n=1}^{m/2} f_n \exp\left[2\pi i(hx_j + \frac{h}{2} + ky_j + \frac{k}{2} + lz_j + \frac{l}{2} \right] \right)$$

While complicated, it is noted that if $h + k + l$ is even, then the second term will contain an integer, n, in it. An integral number of 2π's will have no effect on the value of this term and the equation reduces to:

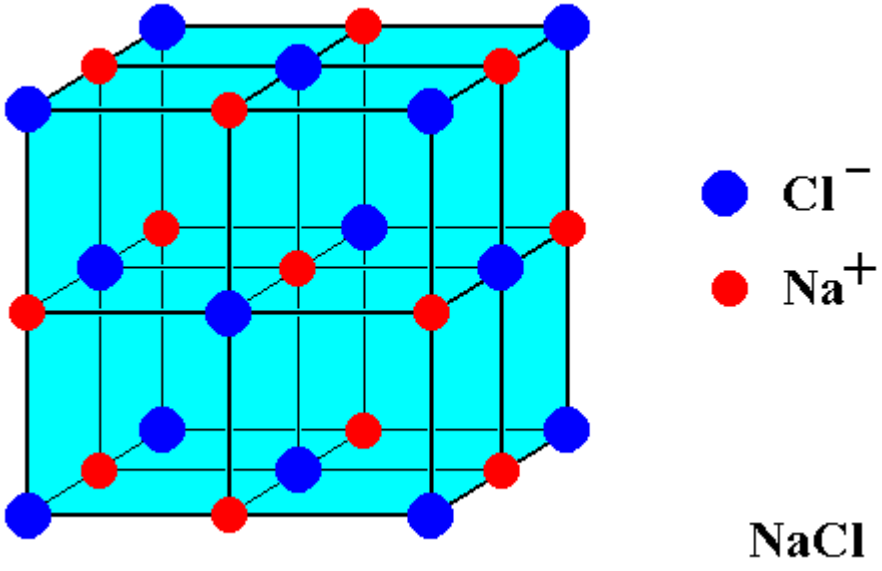
$$\mathbf{F}_{hkl} = \sum_{j=1}^{m/2} 2 f_n \exp\left[2\pi i(hx_j + ky_j + lz_j\right]$$

If $h + k + l$ is odd, however, the second term will contain an integer with a $2\pi(n/2)$ term; here n is any integer and represents a full rotation of the scattering vector. This causes the second term to be negative, and the net result is there is no diffracted intensity (since $\mathbf{F}_{hkl} = 0$). This condition is called a *systematic extinction*. The table below lists the systematic extinction conditions due to translational symmetry elements[1]:

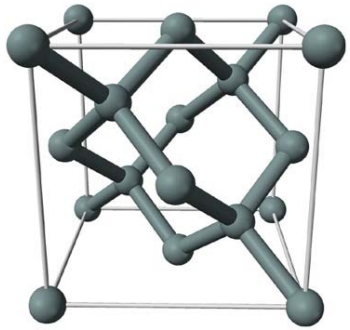
Symmetry	Extinction Conditions
P	none
C	*hkl*; $h + k$ = odd
B	*hkl;* $h + l$ = odd
A	*hkl;* $k + l$ = odd
I	*hkl*; $h + k + l$ = odd
F	*hkl; h, k, l* mixed even and odd
$2_1 \parallel b$	0*k*0: k = odd

P = primitive lattice; C, B, A = side-centered on c-, b-, a-face; I = body centered; F = face centered (001)

question : KCl et NaCl adoptent la même structure (NaCl). Pourtant, le diagramme de diffraction de KCl est plus proche d'un cubique simple que d'un CFC – pourquoi?



simulation du diagramme de diffraction : poudrix (silicium)



POUDRIX (15/11/03)

File Results Erase Help About Quit

Data | X rays | Neutrons | Calcul.

Source: X ray tube

Cell parameters

a	5.43	α	90
b	5.43	β	90
c	5.43	γ	90

System: Cubic, Tetra., Ortho., Hexa.

Select space group

Hermann-Mauguin: FD3M

Hall:

Space Group Nb.:

Experiment

λ	1.54056
2θ1	5
2θ2	110
U	0.001
V	0
W	0.005

Wavelength: Multiple W.L., MoKa1, MoKa2, MoKmoy, MokBet, CuKa1, CuKa2, CuKmoy, CukBet

Th. 2Th Q

Atom coordinates of the asymetric unit

Atom	Lab.	X	Y	Z	B	Pop
Si		0.12500	0.12500	0.12500	1.00	1.000

Anomalous dispersion

Elem.	1.5406 f'	1.5406 f''
Si	0.000	0.000

Read Anomalous Factors

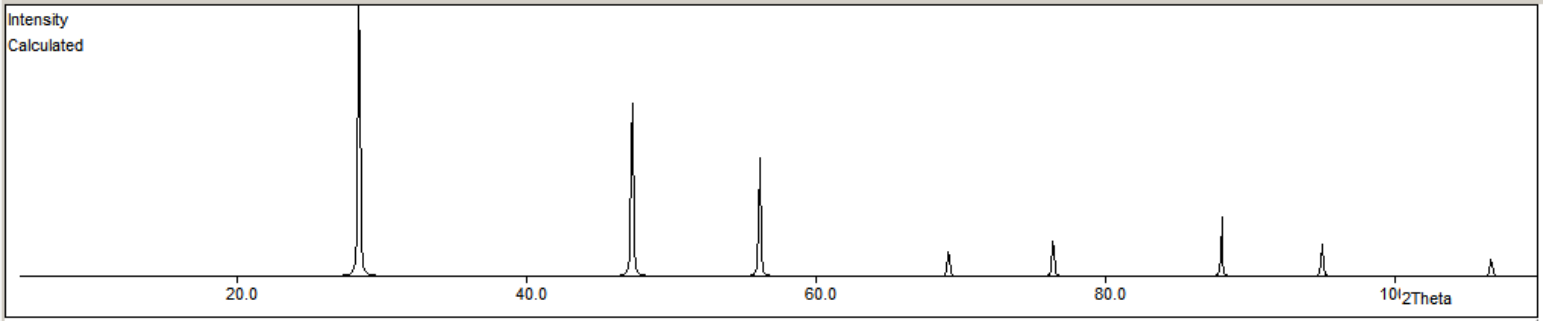
Title:

Results

Nb.	h	k	l	Dhkl	2Theta	k*Int.	lambd
K=	0.0009777						
1	1	1	1	3.1350	28.447	100.0	1.54056
2	2	0	2	1.9198	47.310	61.6	1.54056
3	1	1	3	1.6372	56.131	34.9	1.54056
4	2	2	2	1.5675	58.866	0.0	1.54056
5	0	0	4	1.3575	69.142	8.6	1.54056
6	3	1	3	1.2457	76.390	12.3	1.54056
7	4	2	2	1.1084	88.047	16.2	1.54056
8	1	1	5	1.0450	94.971	6.8	1.54056
9	3	3	3	1.0450	94.971	2.3	1.54056
10	4	0	4	0.9599	106.731	5.6	1.54056

Diffraction diagram

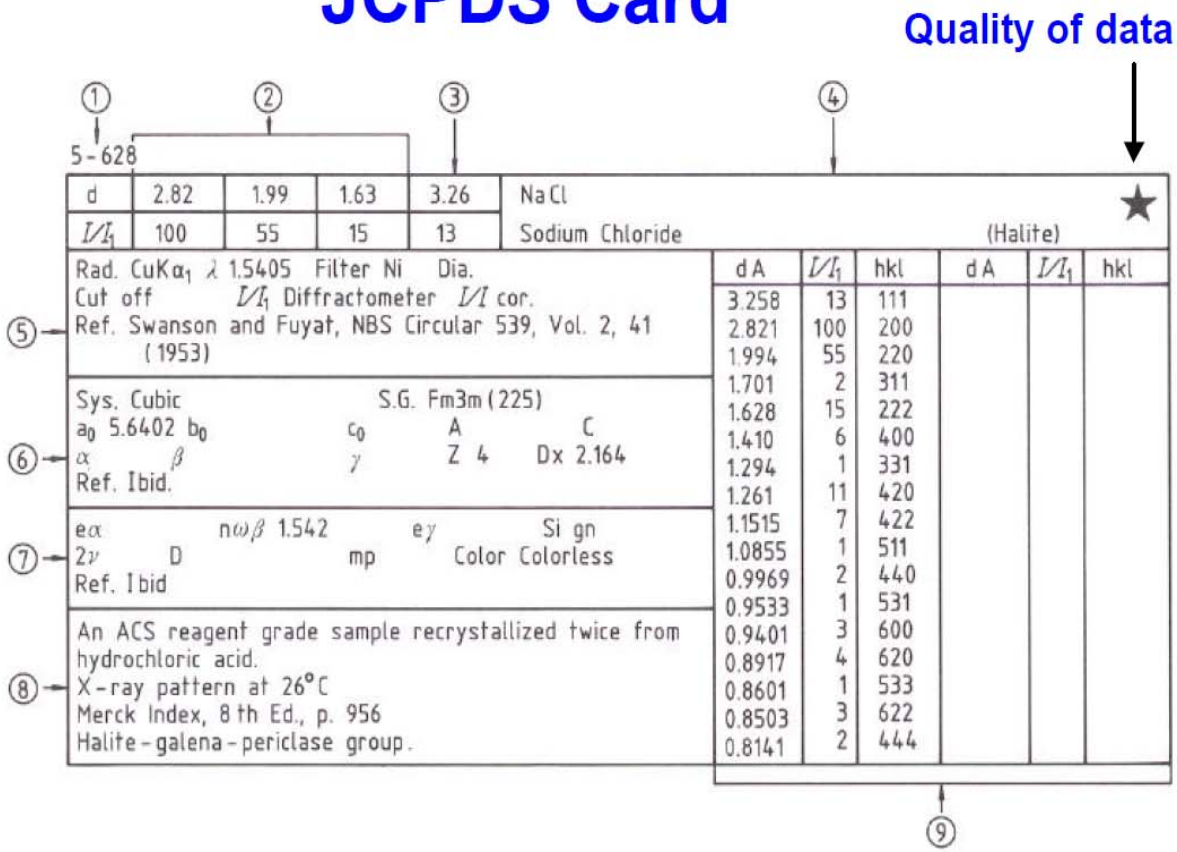
File Y Scale Print Save image Erase Difference Help



2Th= 57.08 d= 1.612

Click on a peak to index it, or click on a line of the list. Click and drag a box to "zoom". Click on the right button to "unzoom".

JCPDS Card

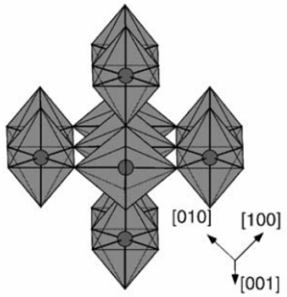


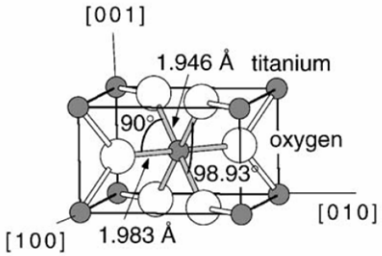
1.file number 2.three strongest lines 3.lowest-angle line 4.chemical formula and name 5.data on diffraction method used 6.crystallographic data 7.optical and other data 8.data on specimen 9.data on diffraction pattern.

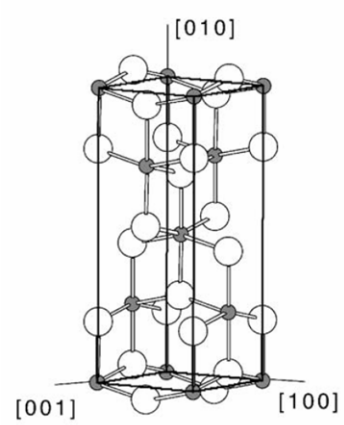
Joint Committee on Powder Diffraction Standards, JCPDS (1969)
Replaced by International Centre for Diffraction Data, ICDF (1978)

Oxyde de titane

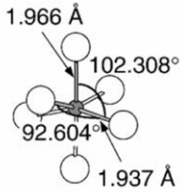
Rutile

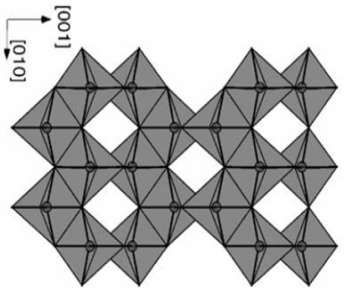


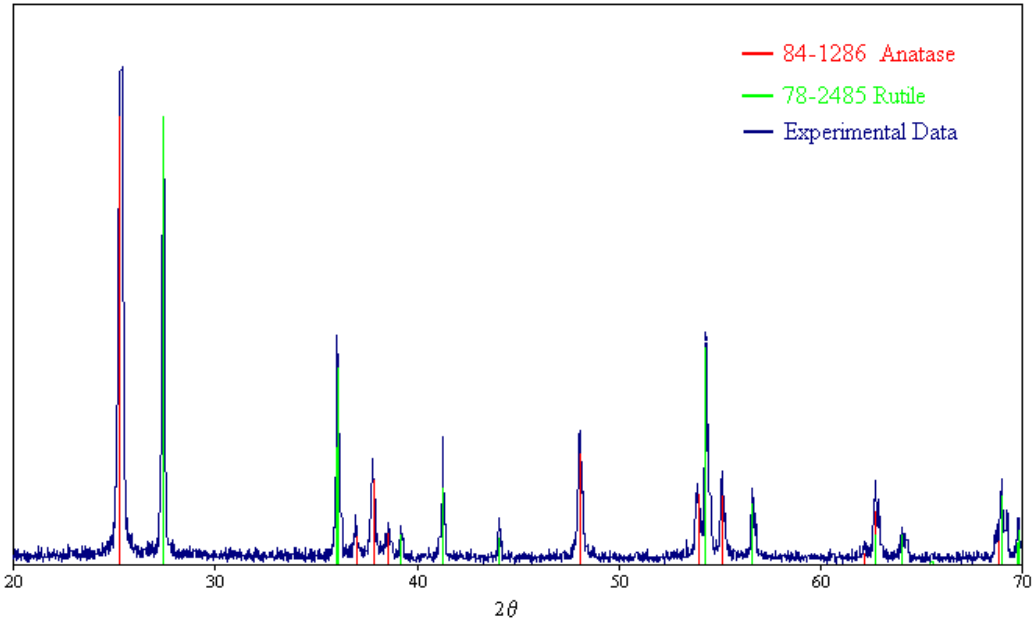




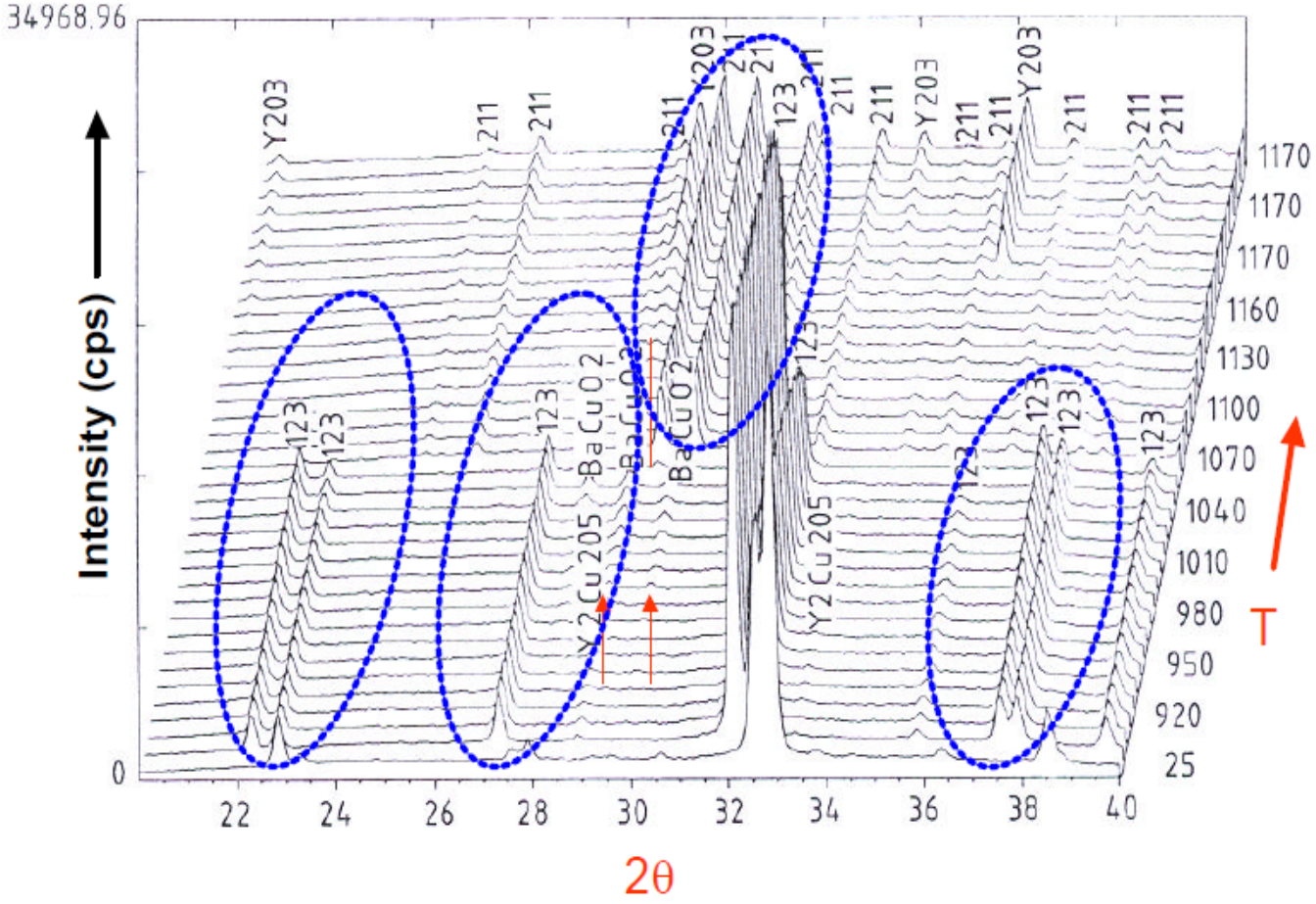
Anatase



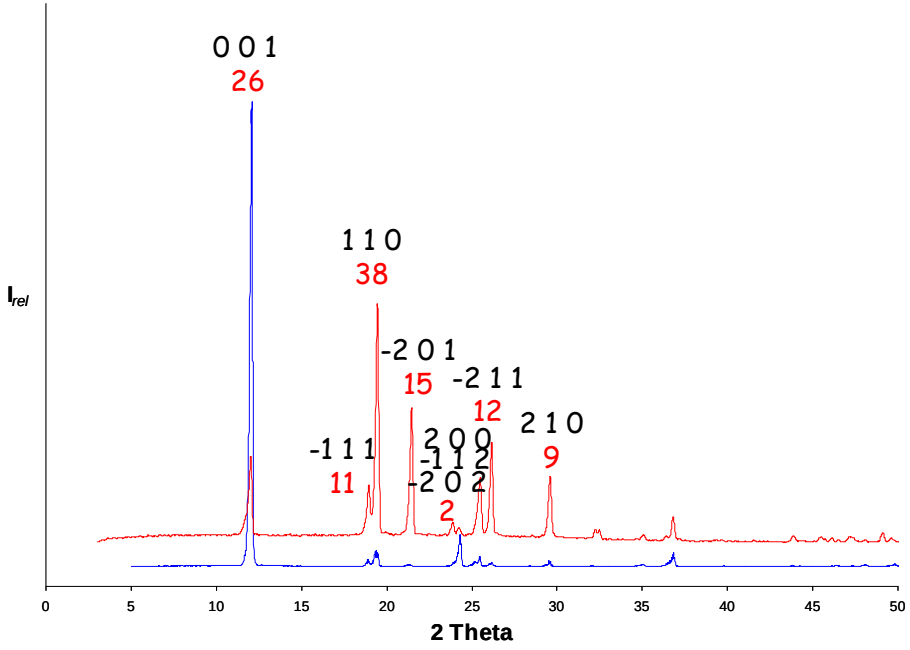


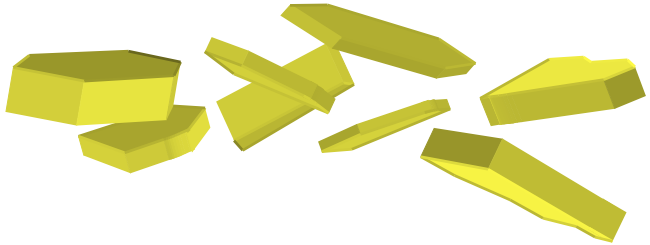


High Temperature XRD Patterns of the Decomposition of $YBa_2Cu_3O_{7-\delta}$

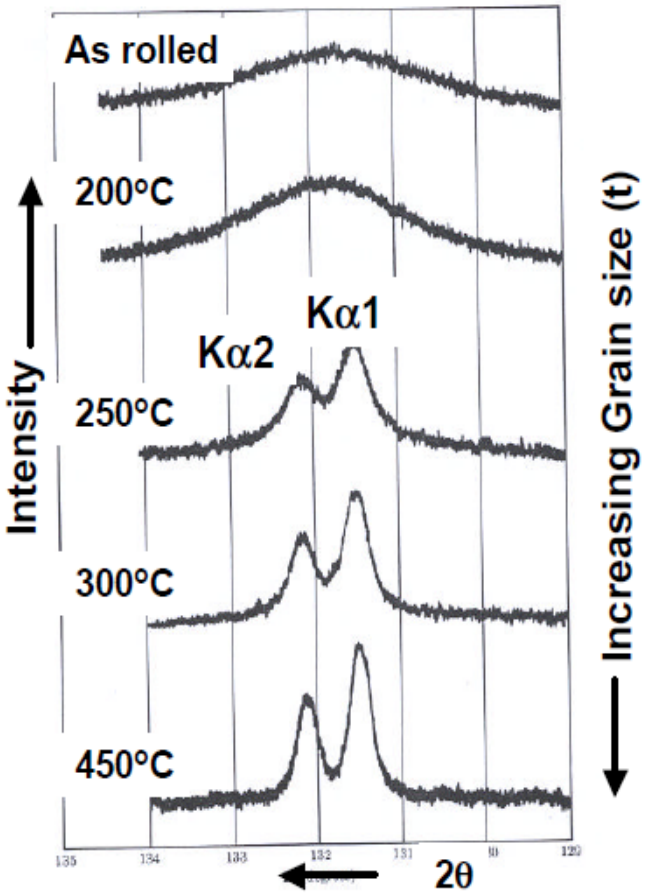


Effet de texturation

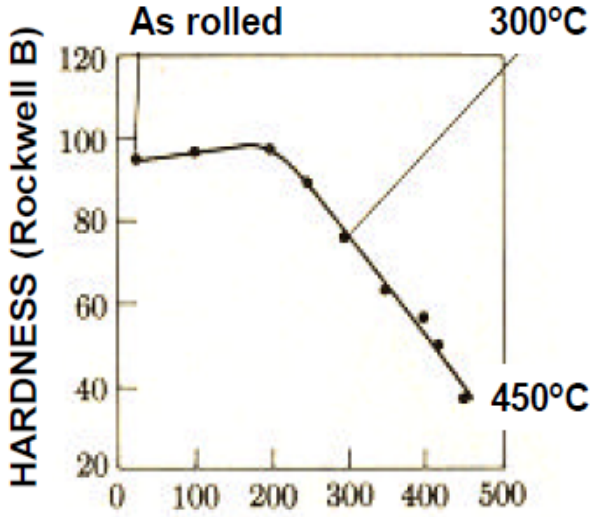




Effect of Coherent Domain Size



(331) Peak of cold-rolled and Annealed 70Cu-30Zn (brass)

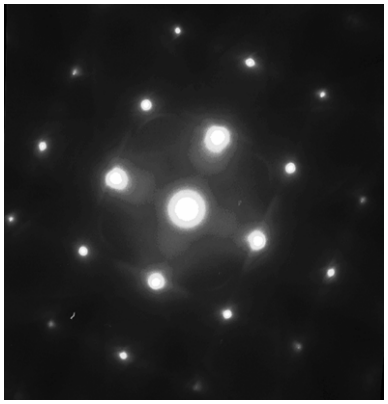


$$B = \frac{0.9 \cdot \lambda}{t \cdot Cos\theta}$$

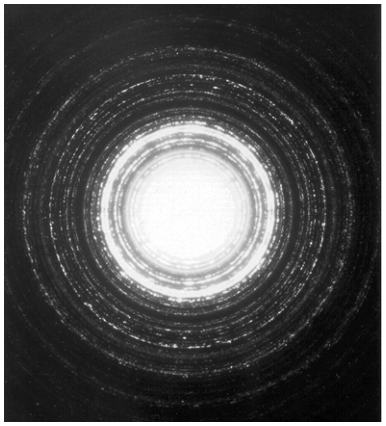
Peak Broadening
Scherrer Model

As grain size decreases hardness increases and peaks become broader

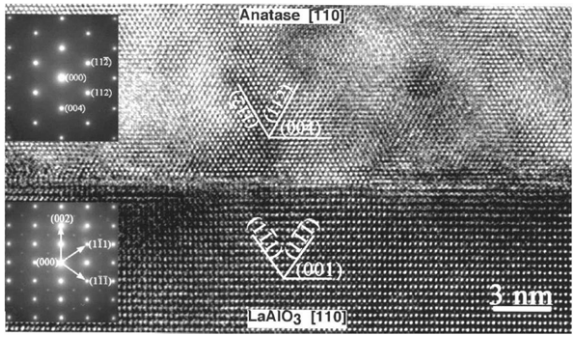
Diffraction électronique

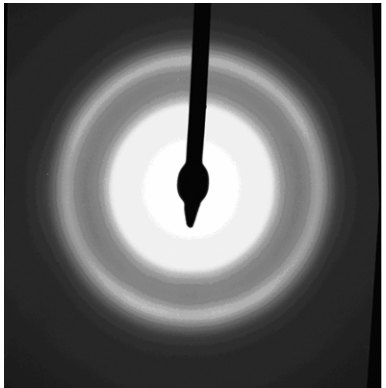


monocristal



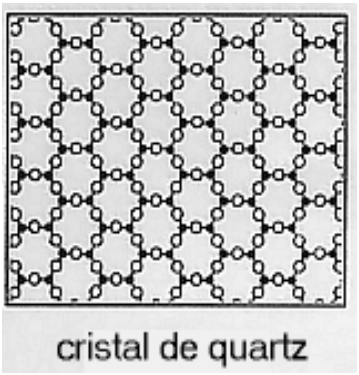
poudre

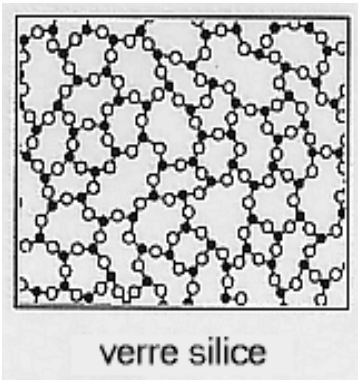


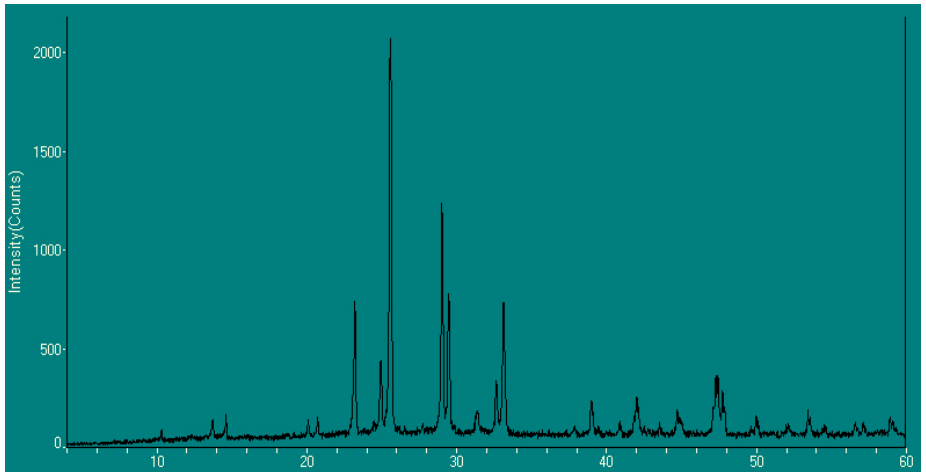


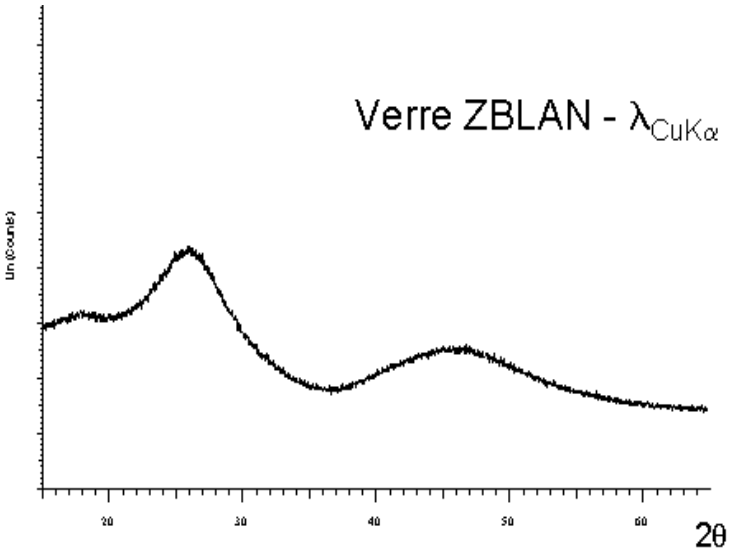
amorphe

diffraction des amorphes









fonction de distribution radiale