X-Ray diffraction patterns of amorphous alloy $Zr_{60}Cu_{20}Fe_{20}$ and their evolution at high temperature

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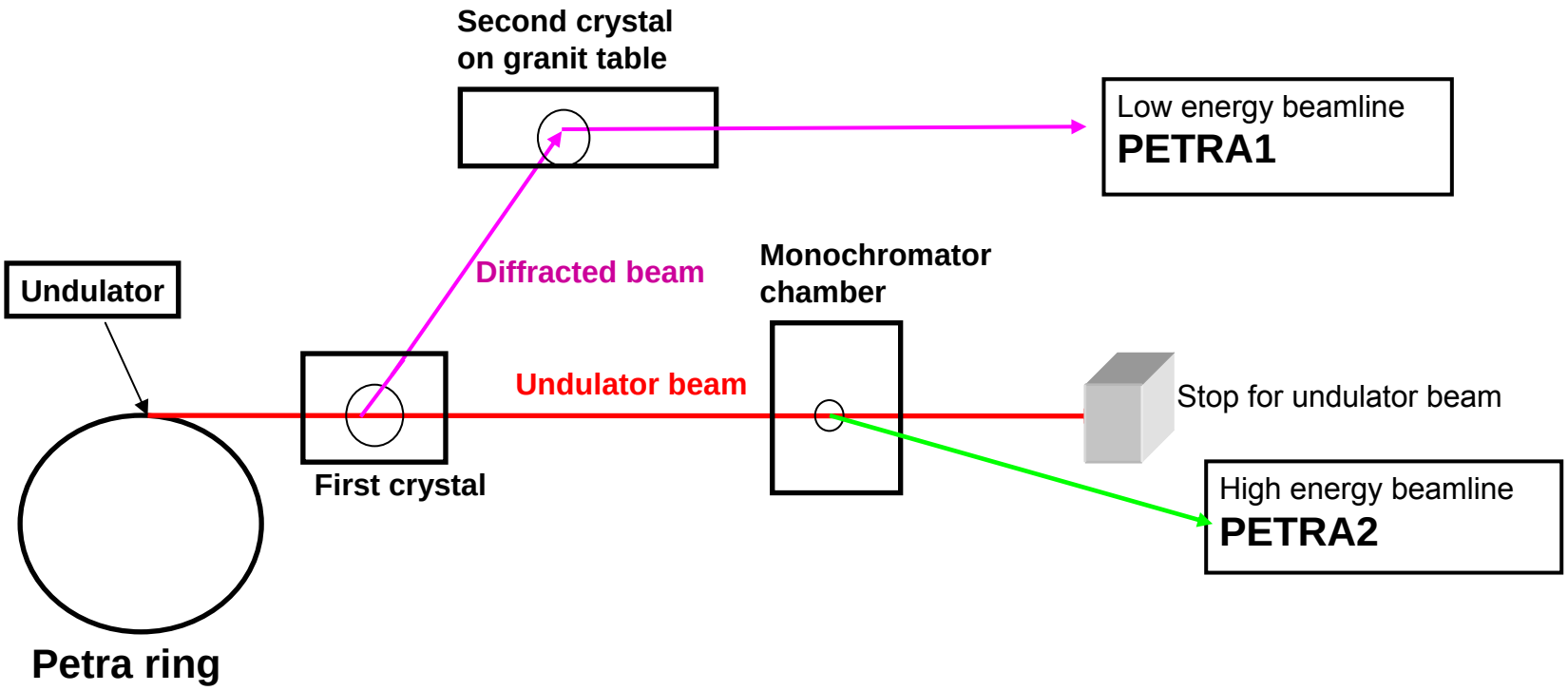
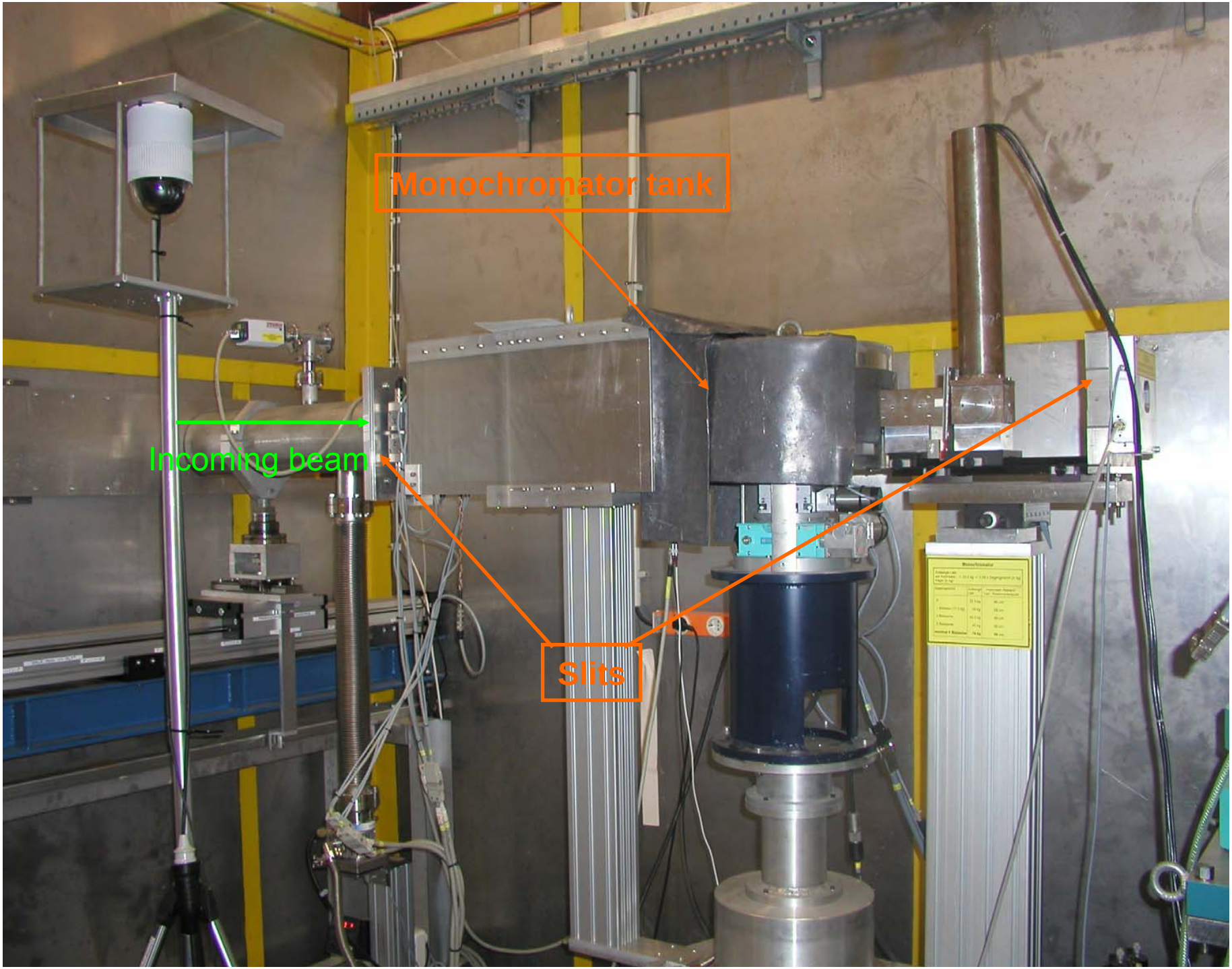
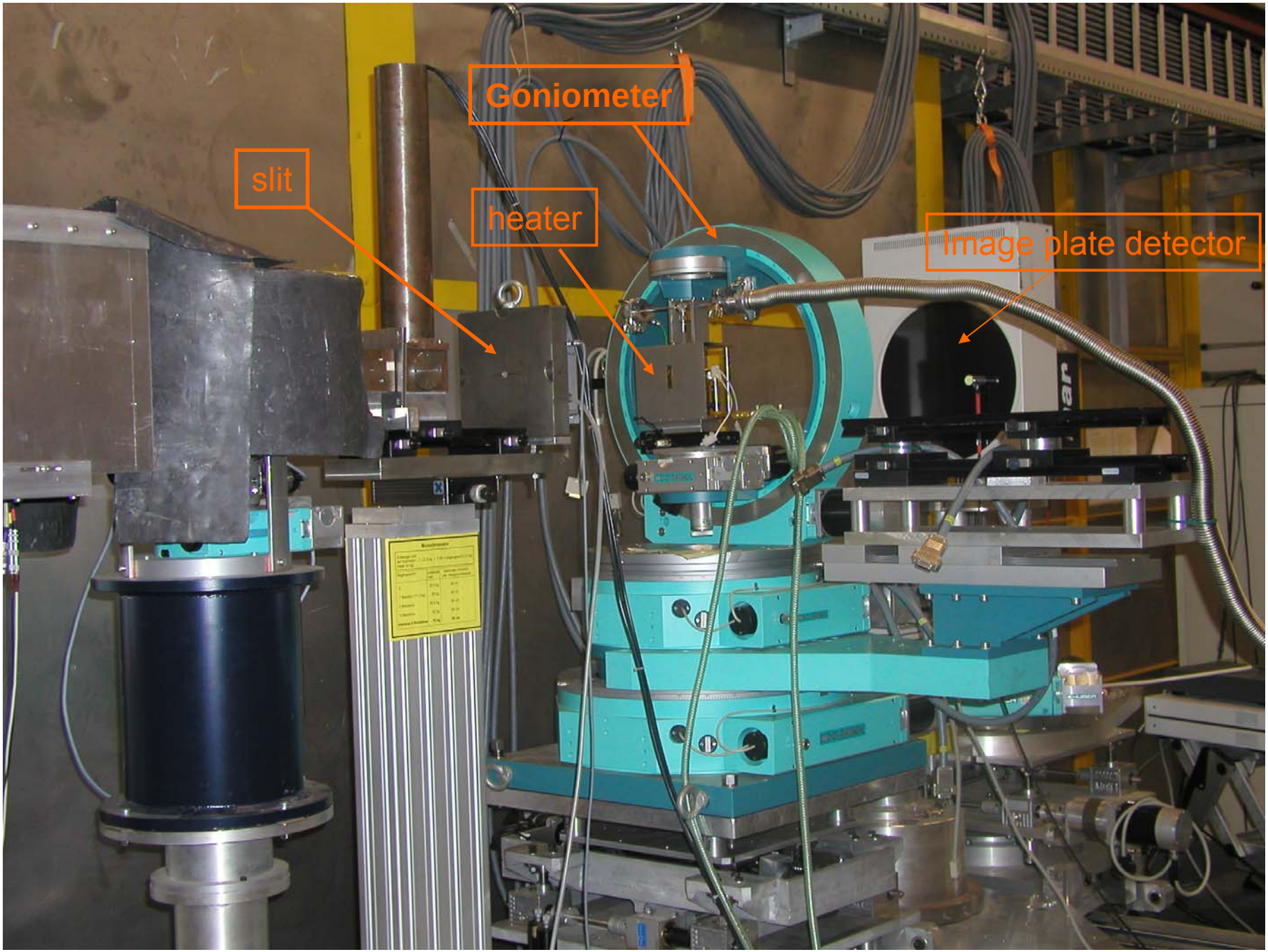
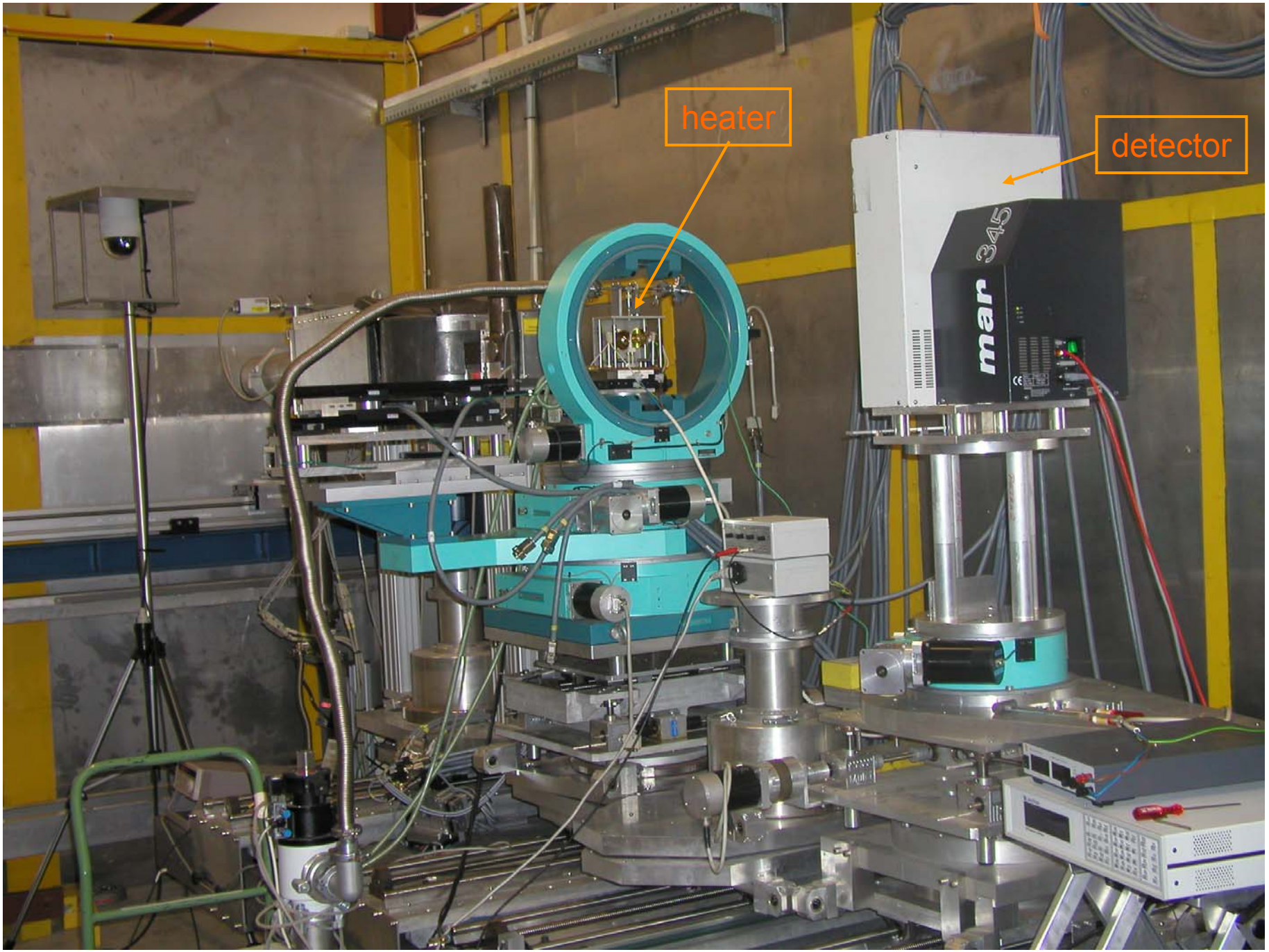
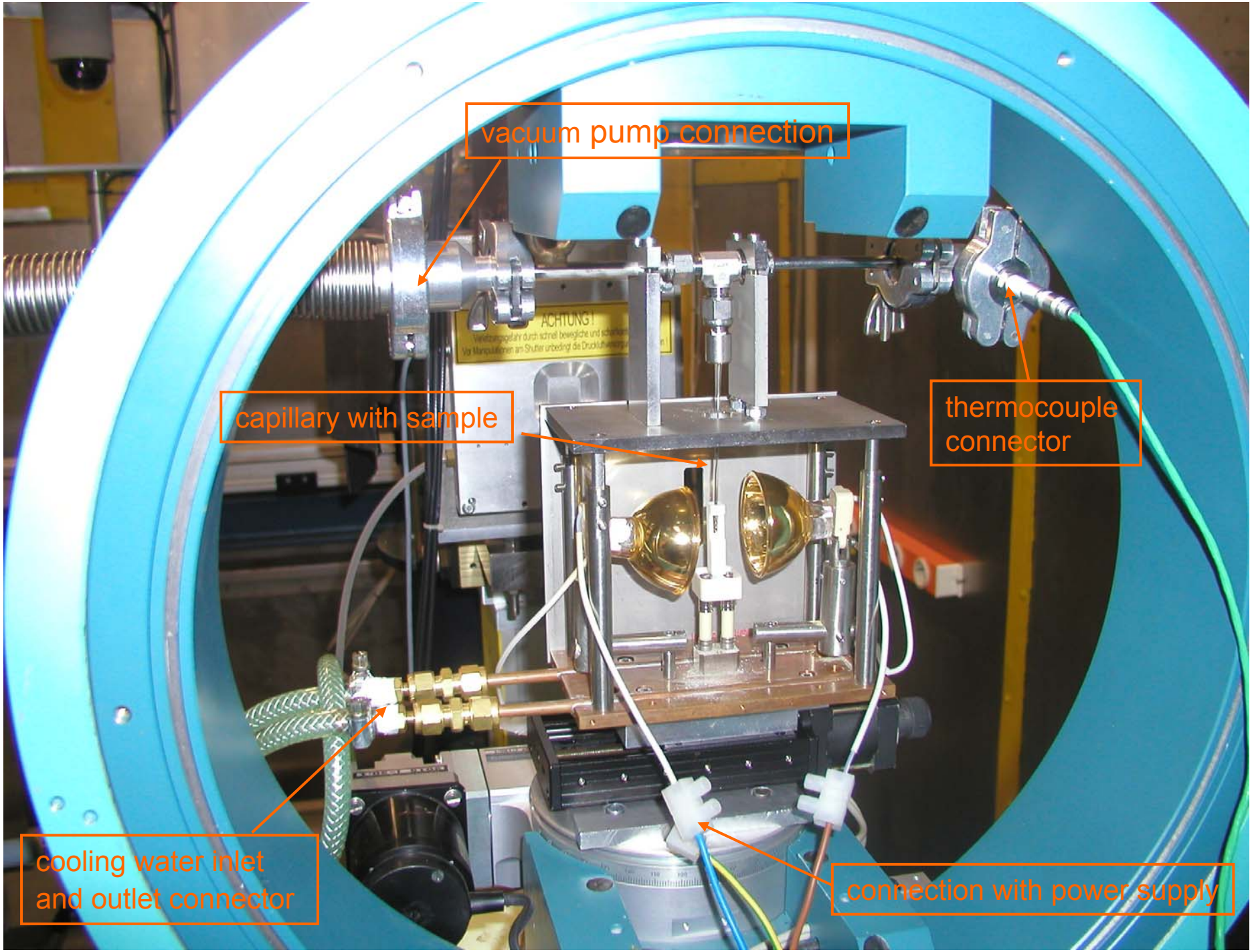
Beamline description



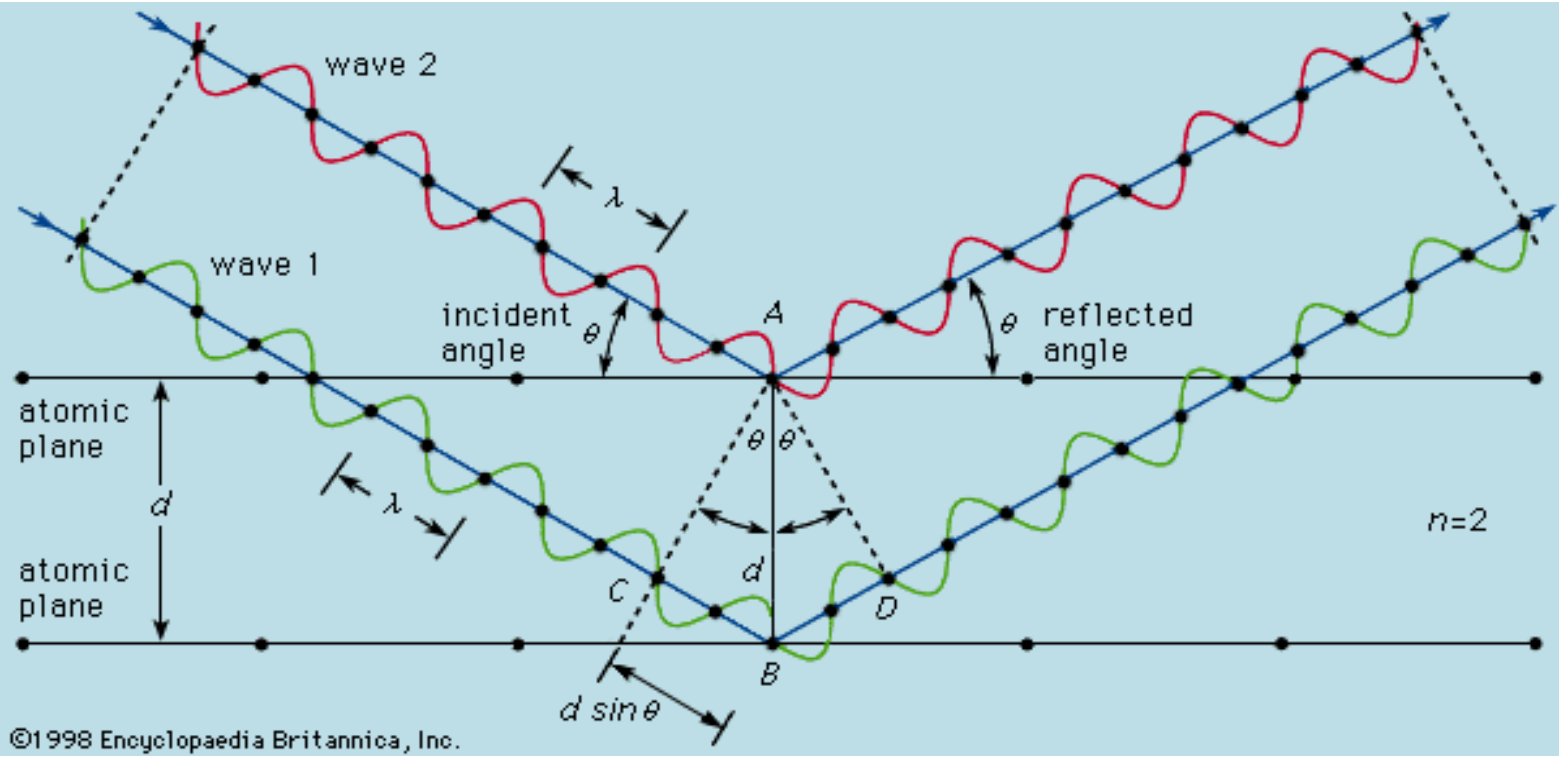

Monochromator tank
Incoming beam
Slits


Goniometer
slit
heater
Image plate detector


heater
detector
mar 345


vacuum pump connection
capillary with sample
thermocouple connector
cooling water inlet and outlet connector
connection with power supply

Bragg's law



$$2d\sin\theta = n\lambda$$

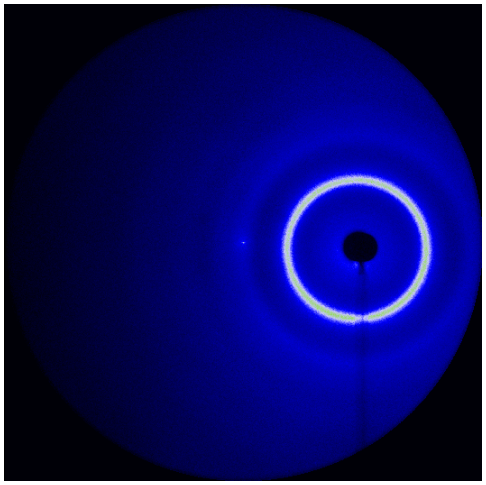
d – spacing between layers of atoms

θ – angle between the incident rays and atomic plane

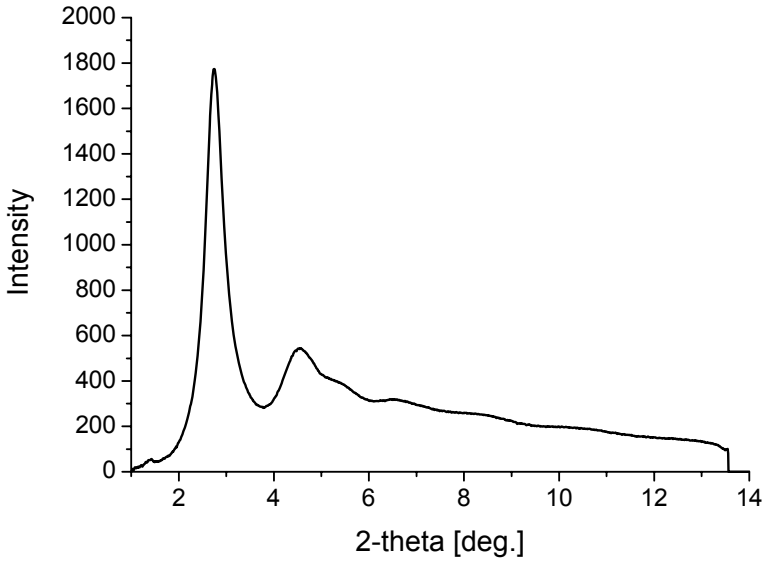
λ – wavelength of radiation

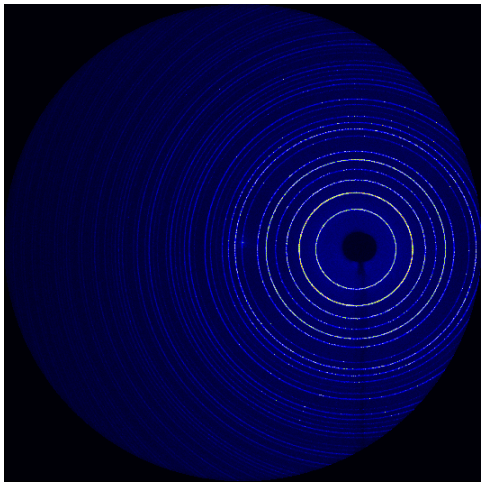
http://www.britannica.com/nobel/micro/83_20.html

X-Ray Diffraction (XRD) patterns from

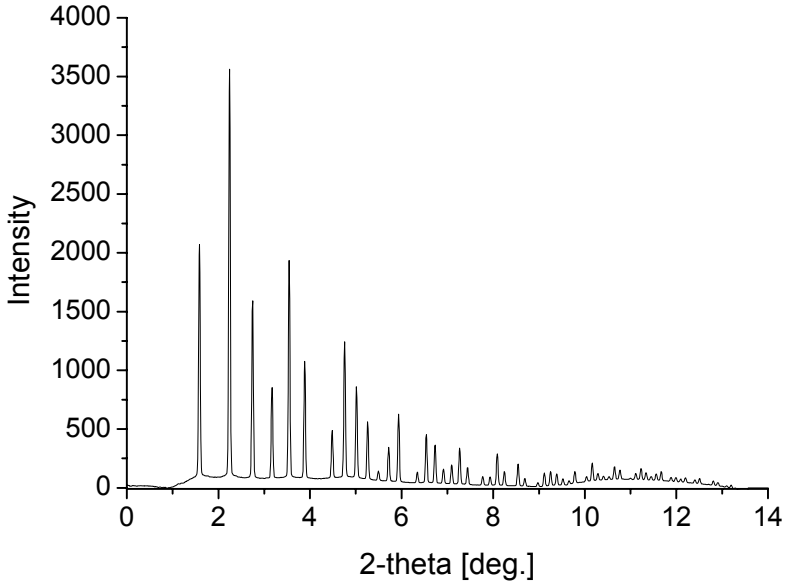


Amorphous alloy
short range order





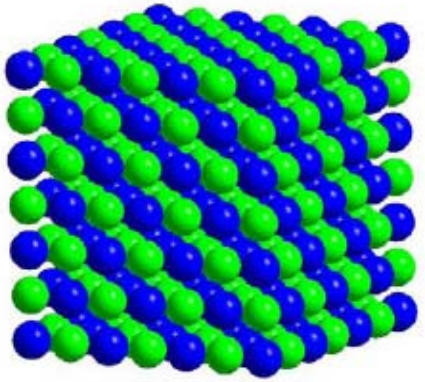
Crystalline alloy
long range order



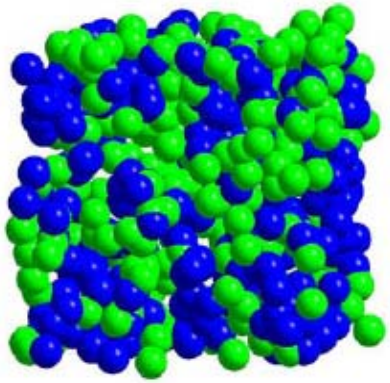
Metallic glasses

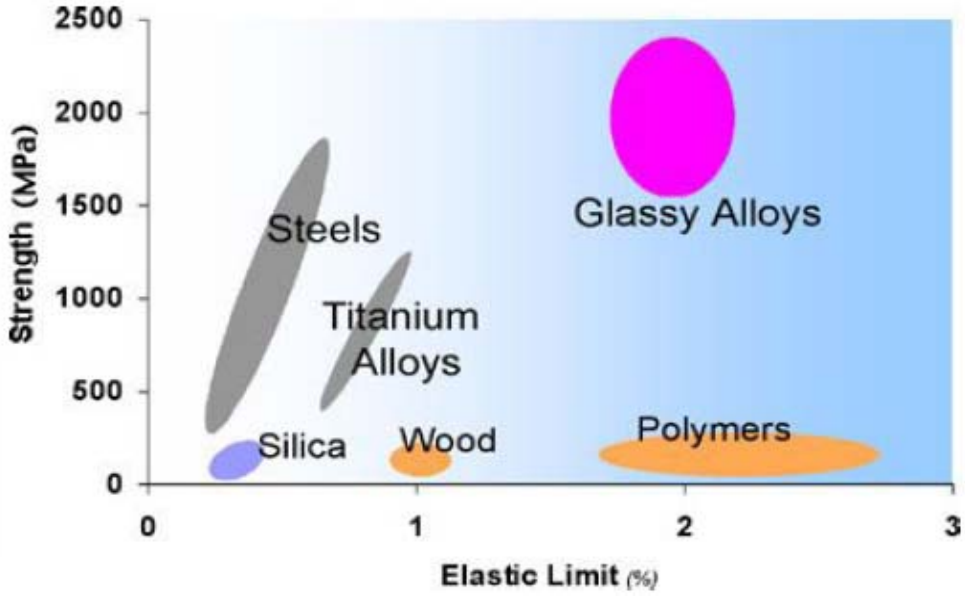
Metallic glasses are a new class of engineering materials having an amorphous structure on atomic level and unlike metals, they can be easily deformed at high temperature.

crystalline



amorphous





Teoretique parts

Calculation of structure factor *S(Q)* by Faber-Ziman formula

$$S(Q) = \frac{I_e(Q) - \langle f^2(Q) \rangle}{\langle f(Q) \rangle^2} \qquad \langle f(Q) \rangle^2 = \left[\sum_\alpha c_\alpha f_\alpha(Q) \right]^2$$

$$\langle f^2(Q) \rangle = \sum_\alpha c_\alpha f_\alpha^2(Q)$$

$I_e(Q)$ – the elastic intensity per atom,

Q – the magnitude of wave vector transfer = $4\pi\sin\theta/\lambda$

λ – the wavelength of scattered radiation

θ – the diffraction angle

$f_\alpha(Q)$ – the atomic form factor

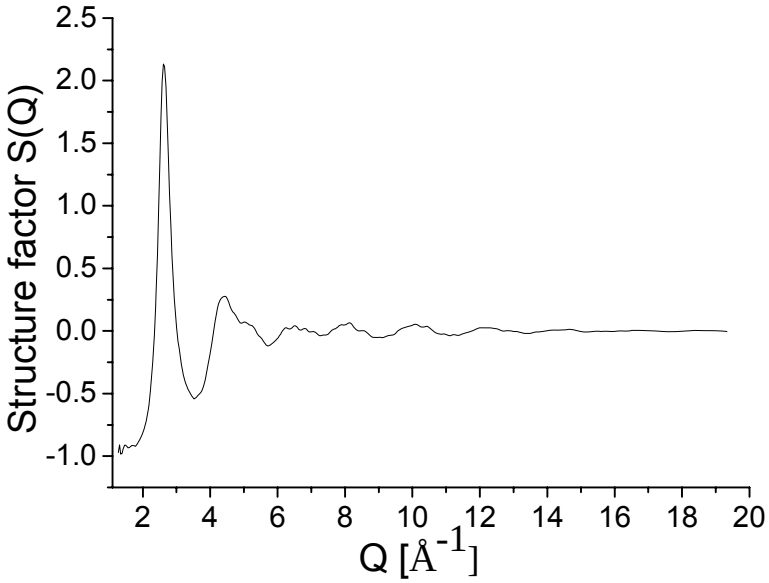
c_α – concentration of particular type of atoms α.

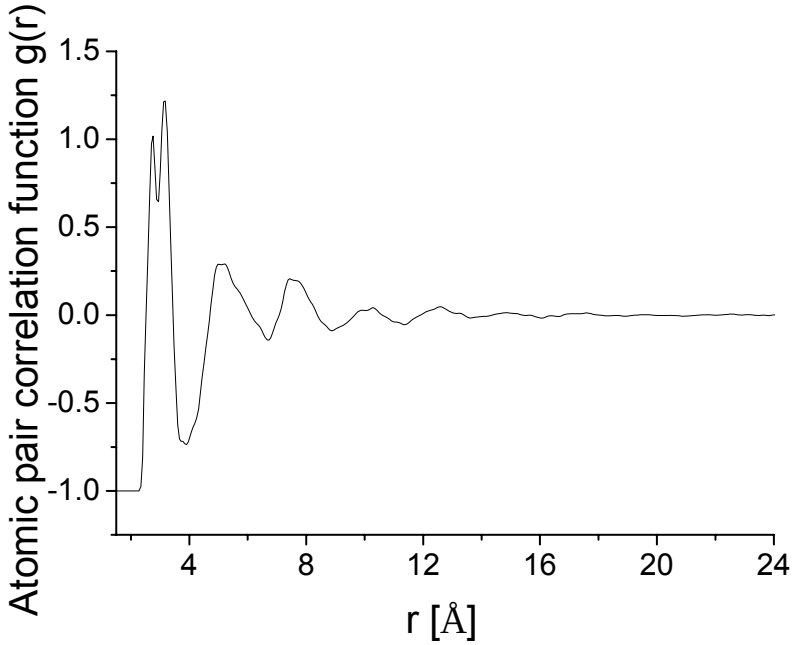
Amorphous structure study of Zr40Cu20Fe20

S(Q)

Fourier transformation

$$g(r) = \frac{2}{\pi}\int_0^{\infty} Q[S(Q)-1]\sin(Qr)dQ$$



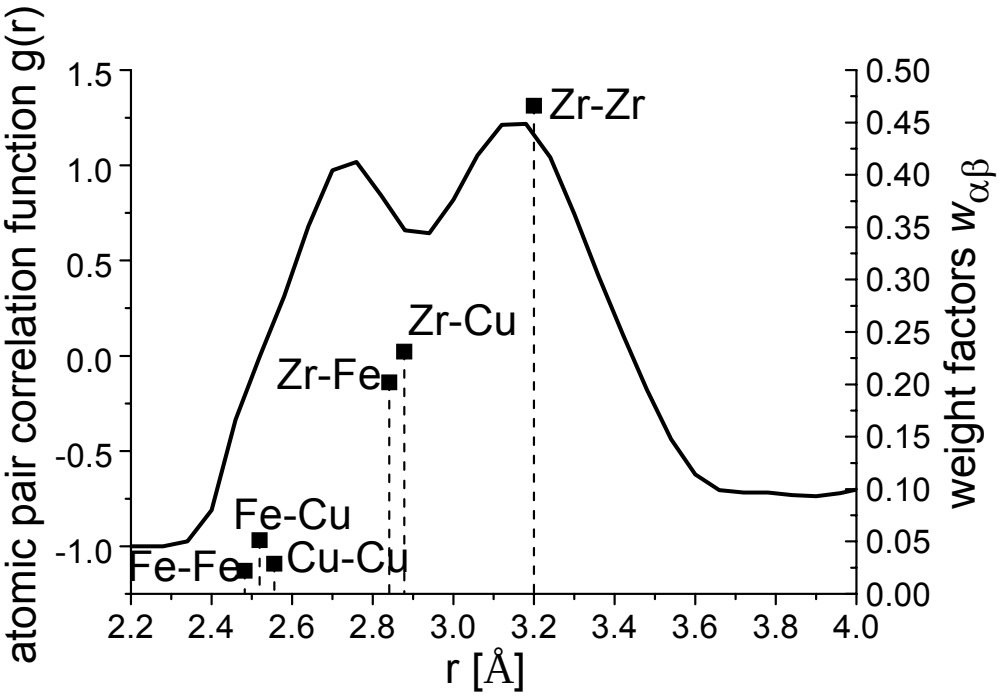


- the shape of S(Q) displays a typical modulation characteristic for conventional metallic glasses

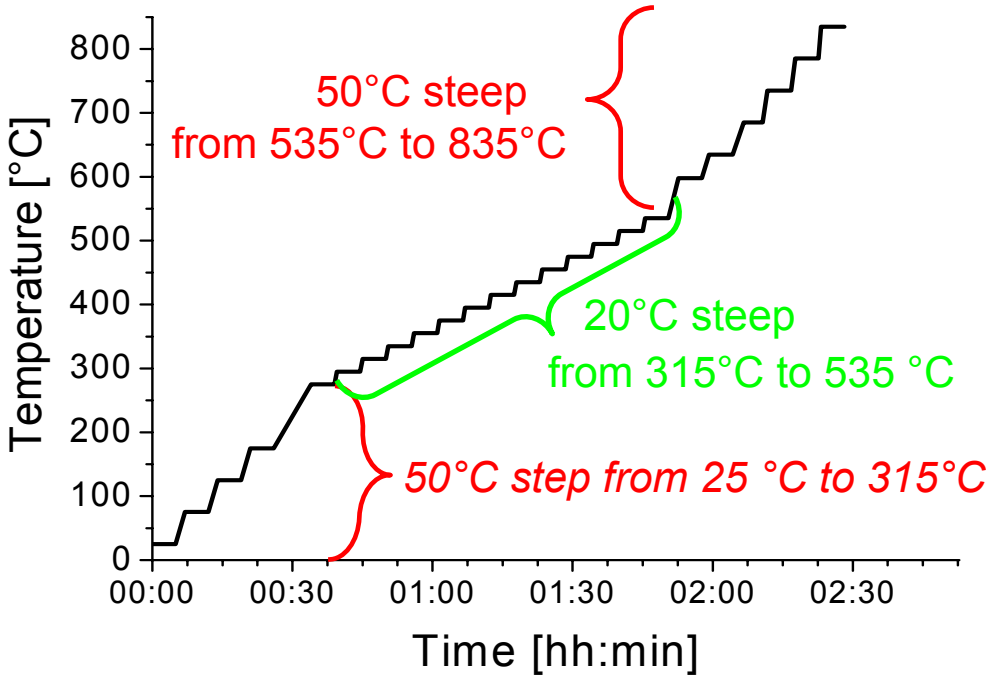
- For three-component alloy (e.g. $Zr_{40}Cu_{20}Fe_{20}$) structure factor *S(Q)* curve consists of the weighted sum of the 6 atomic partial functions *Sij(Q)* with weight factors w_{ij}

$$w_{ij} = c_i c_j f_i f_j \Big/ \left(\sum_i c_i f_i \right)^2$$

Bond type	Distance between two atoms (Å)	Weight factors
Zr-Zr	3.2	0.4668
Zr-Cu	2.878	0.2313
Zr-Fe	2.841	0.2020
Fe-Cu	2.519	0.0513
Cu-Cu	2.519	0.0287
Fe-Fe	2.482	0.0219



High temperature study

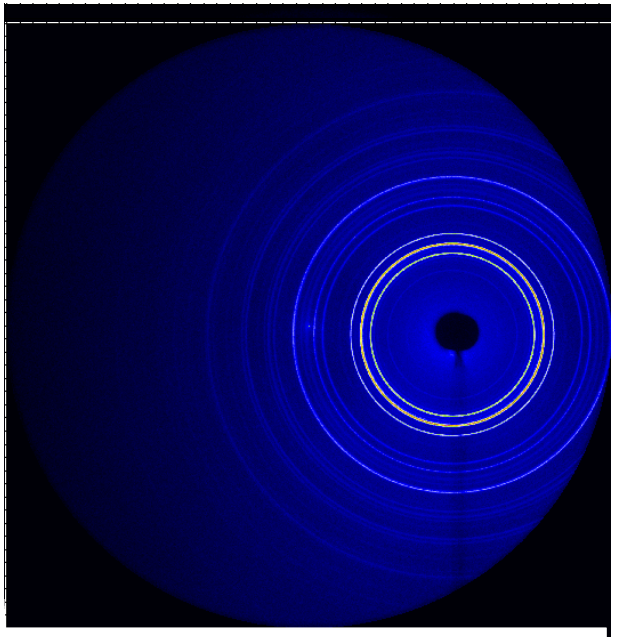


Why ?

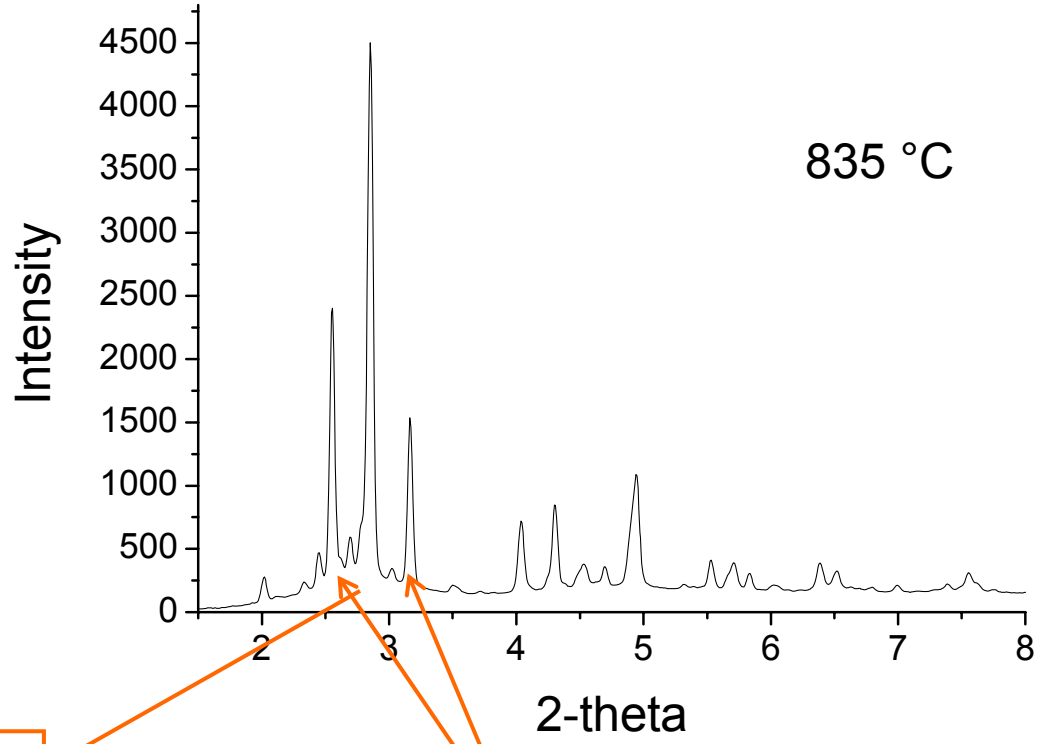
- to know structural evolution at temperature loading

Sketch of tactics at measurement

Evolution of diffraction patterns at temperature loading

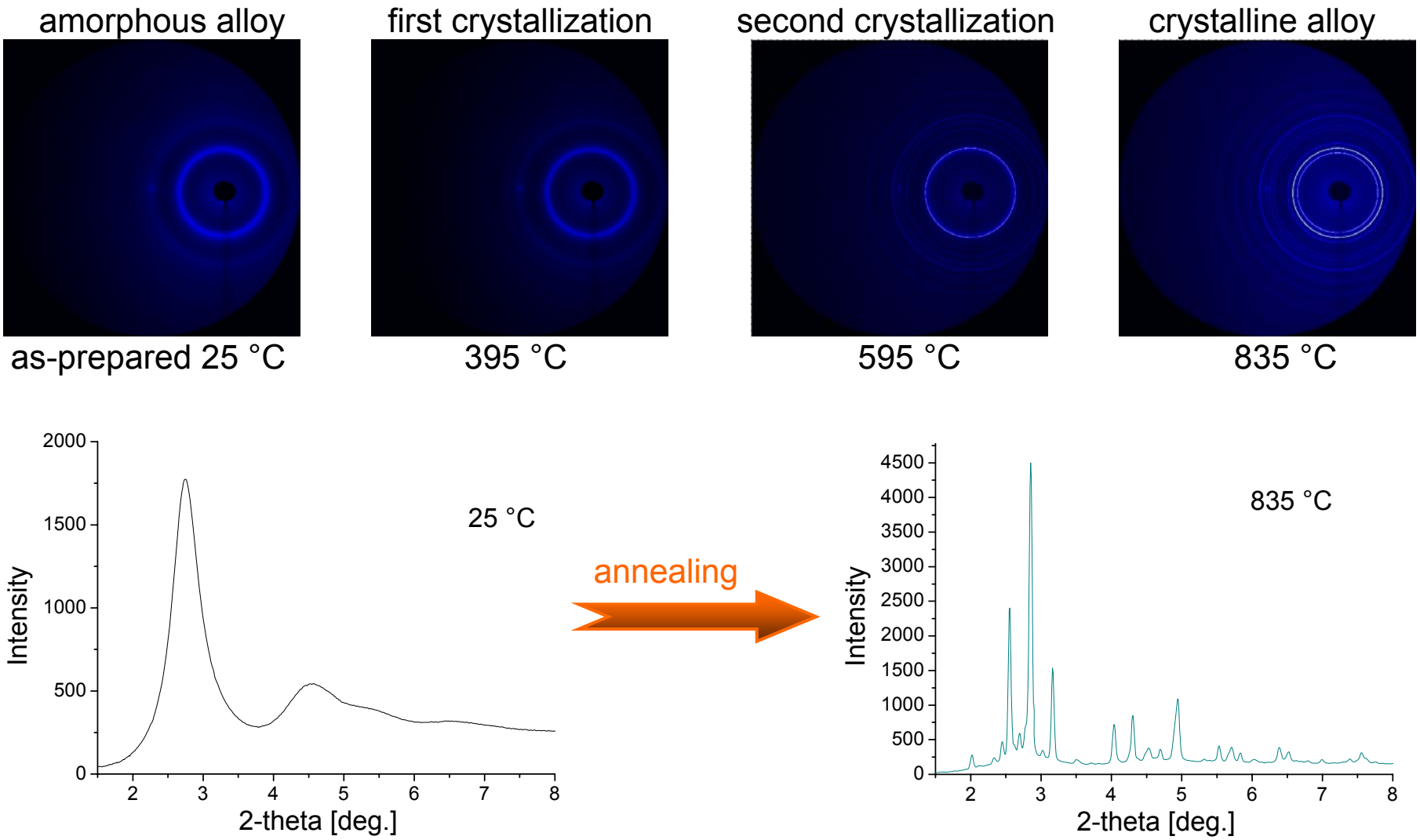


835 °C

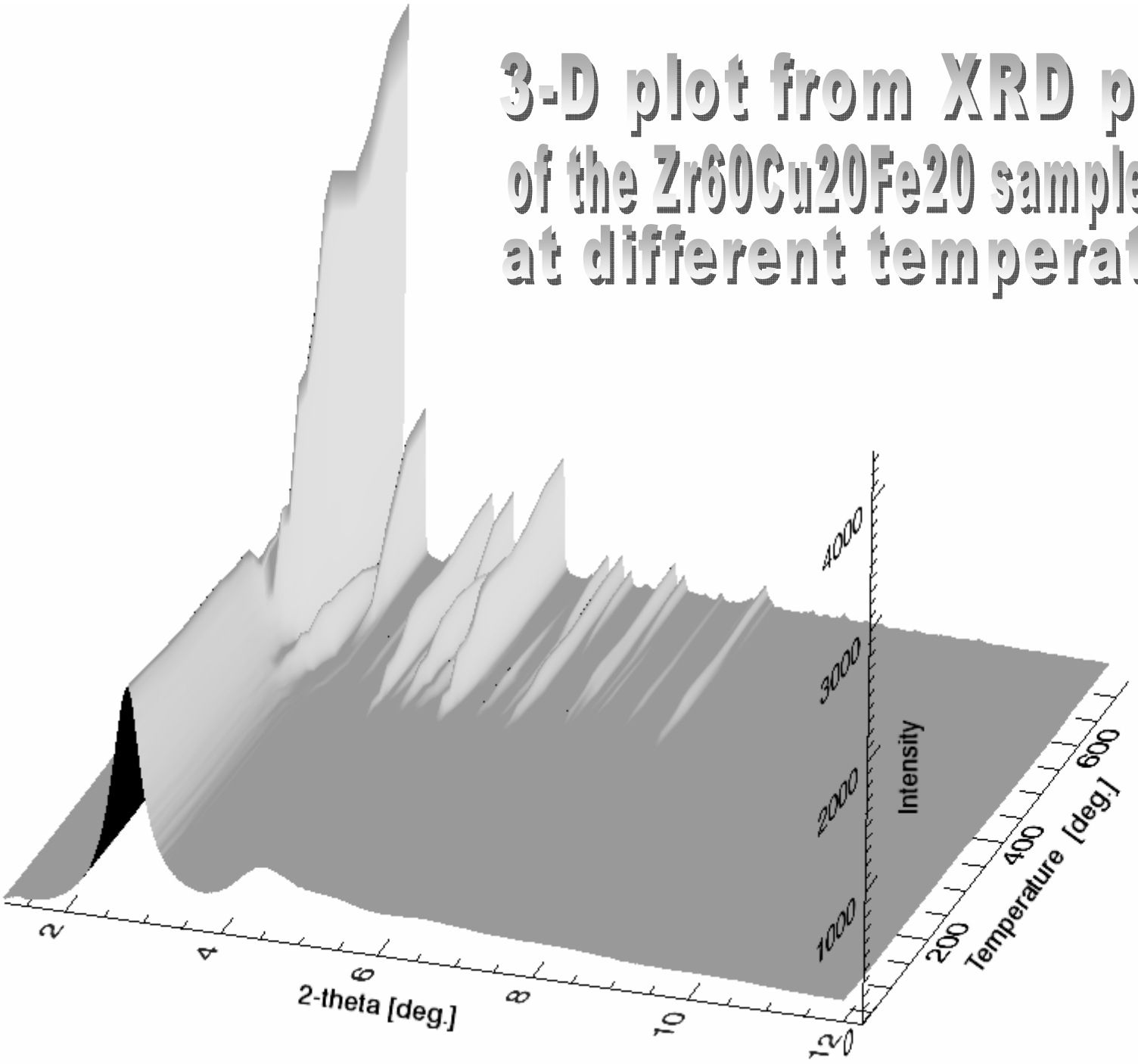


Bragg's peak are appearing

Additional Bragg 's peaks

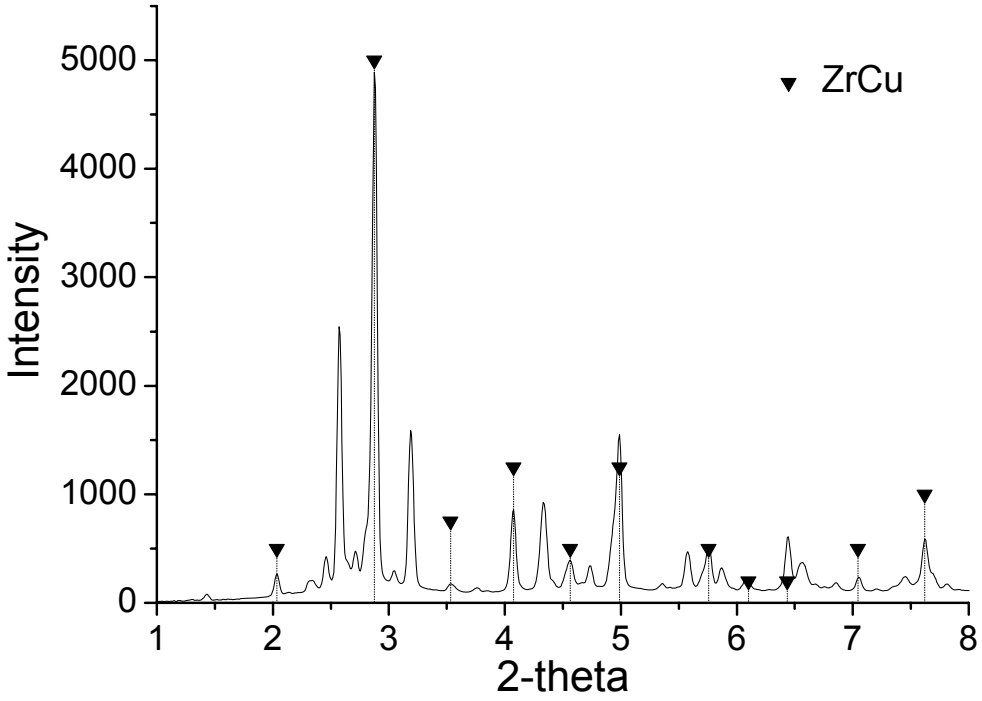

amorphous alloy
first crystallization
second crystallization
crystalline alloy
as-prepared 25 °C
395 °C
595 °C
835 °C
Intensity
2-theta [deg.]
25 °C
annealing
835 °C

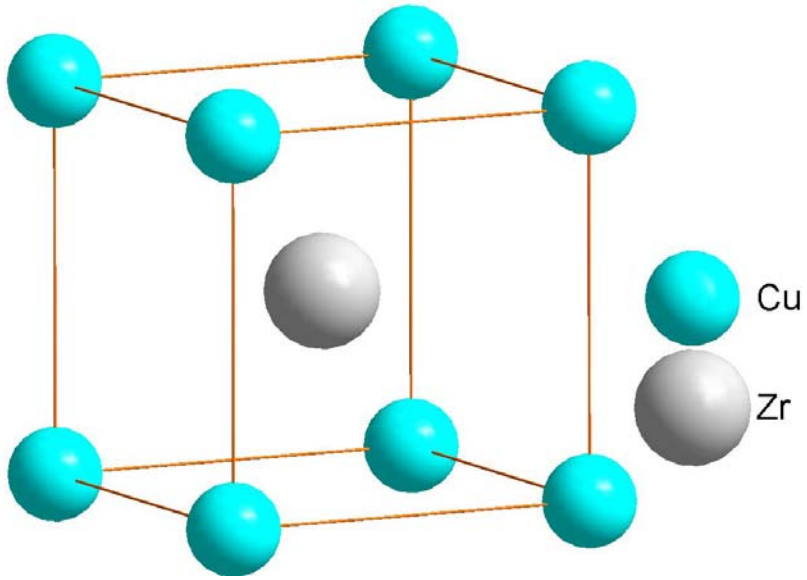
3-D plot from XRD patterns of the Zr60Cu20Fe20 sample annealed at different temperatures



2-theta
2
4
6
8
10
12
temperature [°C]
200
400
600
1000
2000
3000
4000

The phase analysis





- performed on XRD pattern taken from the sample which undergoes the whole temperature cycle and was cooled down to room temperature
- revealed at least a presence of two phases
- indexed only cubic ZrCu phase, having a lattice parameter a = 3.235 Å and space group S.G: $Pm\bar{3}m$