



Unleash the  
**value!**

**ThermoFisher**  
SCIENTIFIC

7<sup>th</sup> workshop

“ Combined analysis examples using X-Ray Scattering”

- Dr. Henry PILLIERE  
(Artenay, France)

**Presentation of ThermoFisher X-ray part (very quick)**

**Interaction X-ray and matter (no maths)**

**Instrumental function**

**XRD setup : some instruments and the information they give**

- **Laboratory systems**
- **Industrial (on-line)**

**Some real XRD examples :**

- **Dust analysis**
- **Phase transition at (not very) high temperature**
- **Thin layer : diffraction, reflectometry, stress**
- **Micro-diffraction**
- **SAXS**

## Global Scale

- 50,000 employees in 50 countries
- \$17 billion in annual revenues
- Unparalleled commercial reach

## Unmatched Depth

- Leading innovative technologies
- Applications expertise
- Lab productivity partner

## Premier Brands

**Thermo**  
SCIENTIFIC

**Invitrogen**

**F** **Fisher**  
**Scientific**

**applied biosystems**

**Unity** Lab Services



## Thermo Fisher Scientific – XRD research

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## Key figures

Creation : 1974 of INEL SAS

INEL integrates Thermo Fisher in Feb. 2016

Staff 2015 : 20 employees 80% technically qualified

(PhD, Engineers and technicians)

Staff seniority average: 10 years

## Resources

All technical and human resources are situated in our headquarter in France :

- Research & Development, technical assistance
- Informatics tools development & assistance
- Mechanical parts design & metrology
- X-Ray diffraction systems assembling
- Installation & After Sales Services for instrumentation
- Components and electronic cards design & integration



# XRD-XRF product portfolio: strong, complementary technologies

## EDXRF



**ARL QUANT'X**  
Top performance  
EDXRF

## WDXRF

**ARL PERFORM'X**  
High performance XRF



**ARL OPTIM'X** – 50W/200W  
Amazing WDXRF

## Integrated XRF and XRD



**ARL 9900 Series**  
Integrated XRF-XRD

## Powder XRD



**ARL X'TRA**



**EQUINOX XRD**

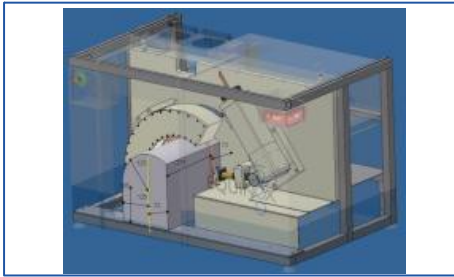
*More on [www.thermoscientific.com/xray](http://www.thermoscientific.com/xray)*



## Instrumentation

Inel designs, manufactures and provides analytical instrumentation:

- X-Ray diffraction instrumentation
- X-Ray radiography instrumentation (CND)
- Extreme Ultraviolet sources instrumentation



## Engineering

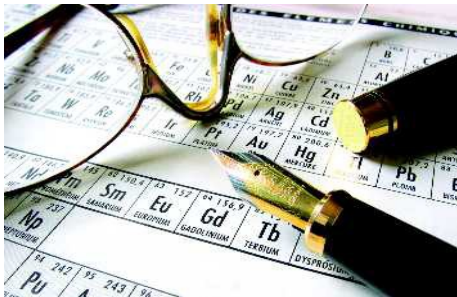
Your needs are specific or evolved and your equipment doesn't fit your needs anymore? Our mission:

- Project consultant & management
- Feasibility studies
- New equipment design & installation

## Scientific Studies & Projects

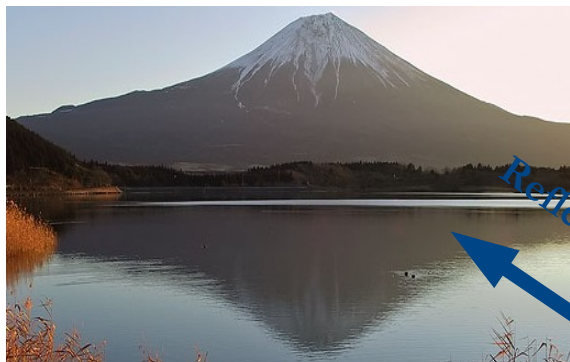
INEL participates in the European and local scale to various projects of R&D to develop Technology.

- European ENVIROMONITOR project coordination: real time automated instrument development using XRD for on-site quantitative analysis on breathable spray particles, including nanoparticles
- Scientific state projects, Thesis financing
- Works coordination & supervision
- Patents creation & operation
- SolXpert project, granted by Région Centre (Fr)
- SOLSA project H2020 raw material



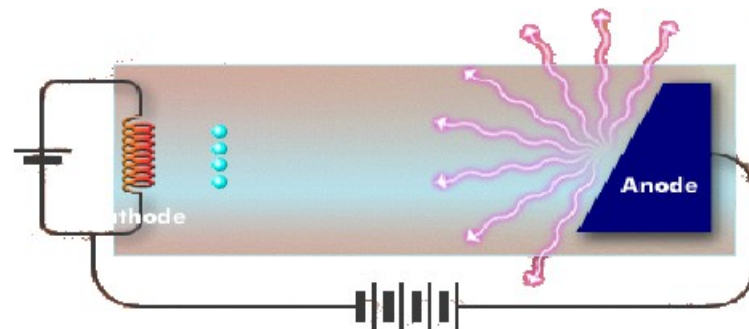
**... and radiation always  
interact with matter ...**

# Wave-matter interaction

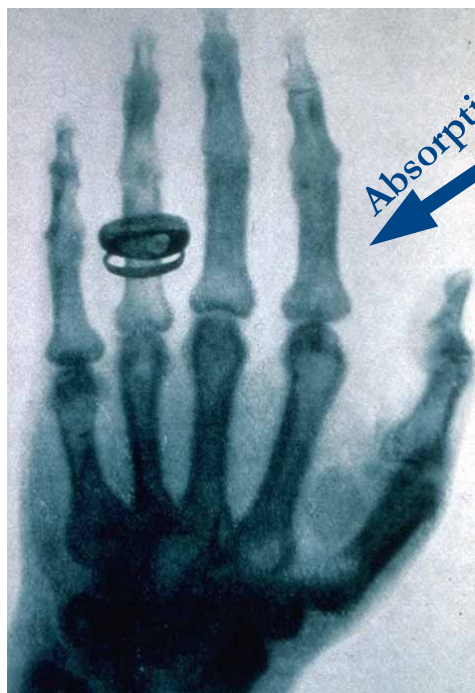


Reflection

**X-rays Production** : classically by excitation of external electronic level with electron beam

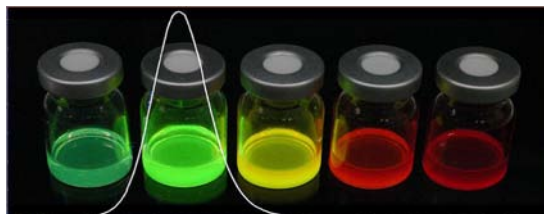


Diffusion

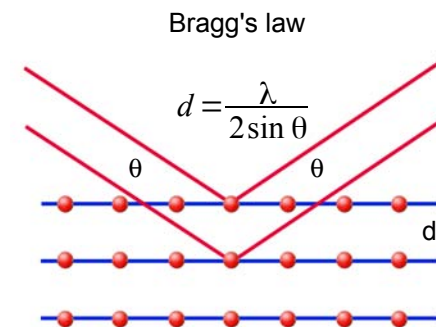


Absorption

fluorescence



Diffraction

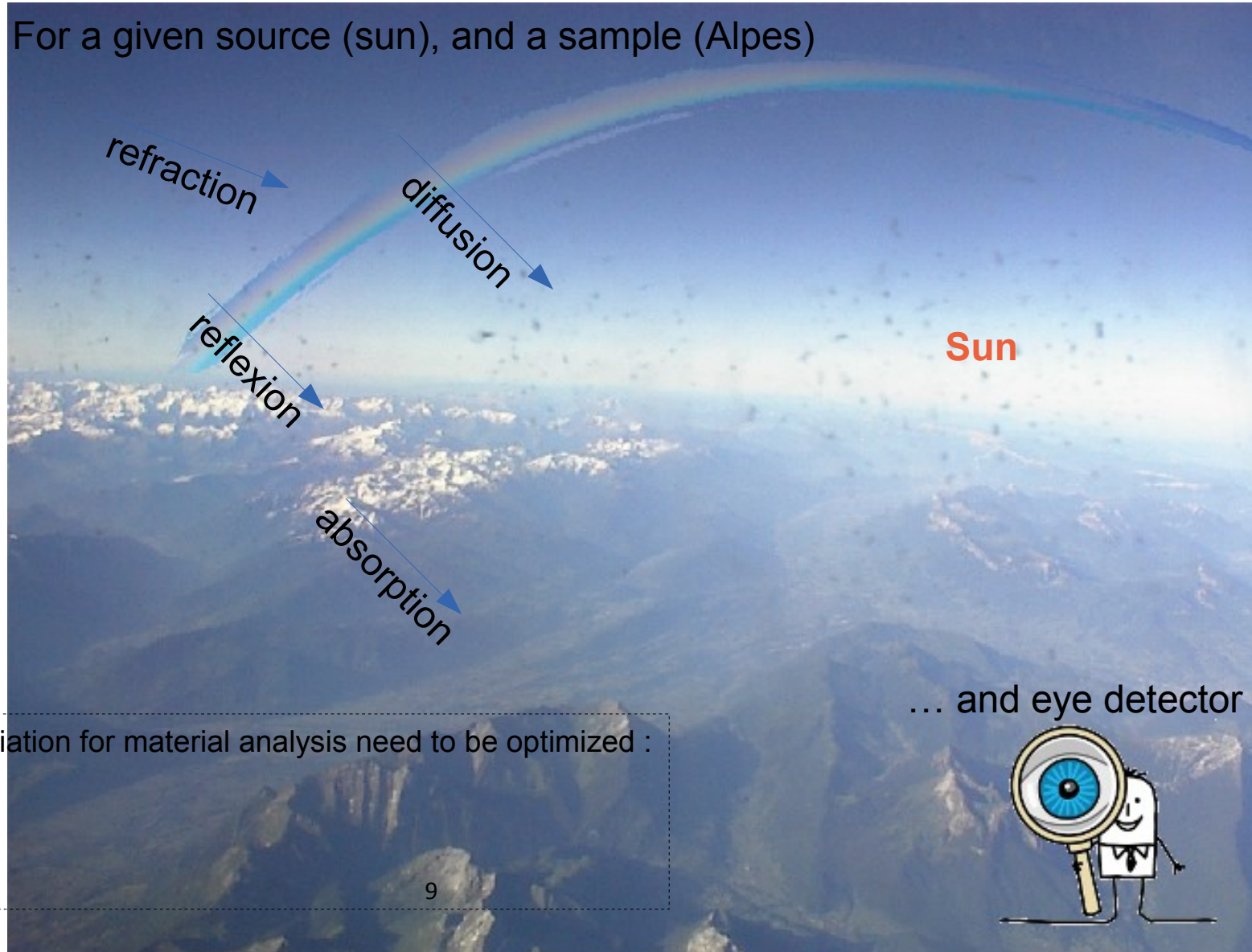




# Interaction wave-matter

Who can see the error?

For a given source (sun), and a sample (Alpes)

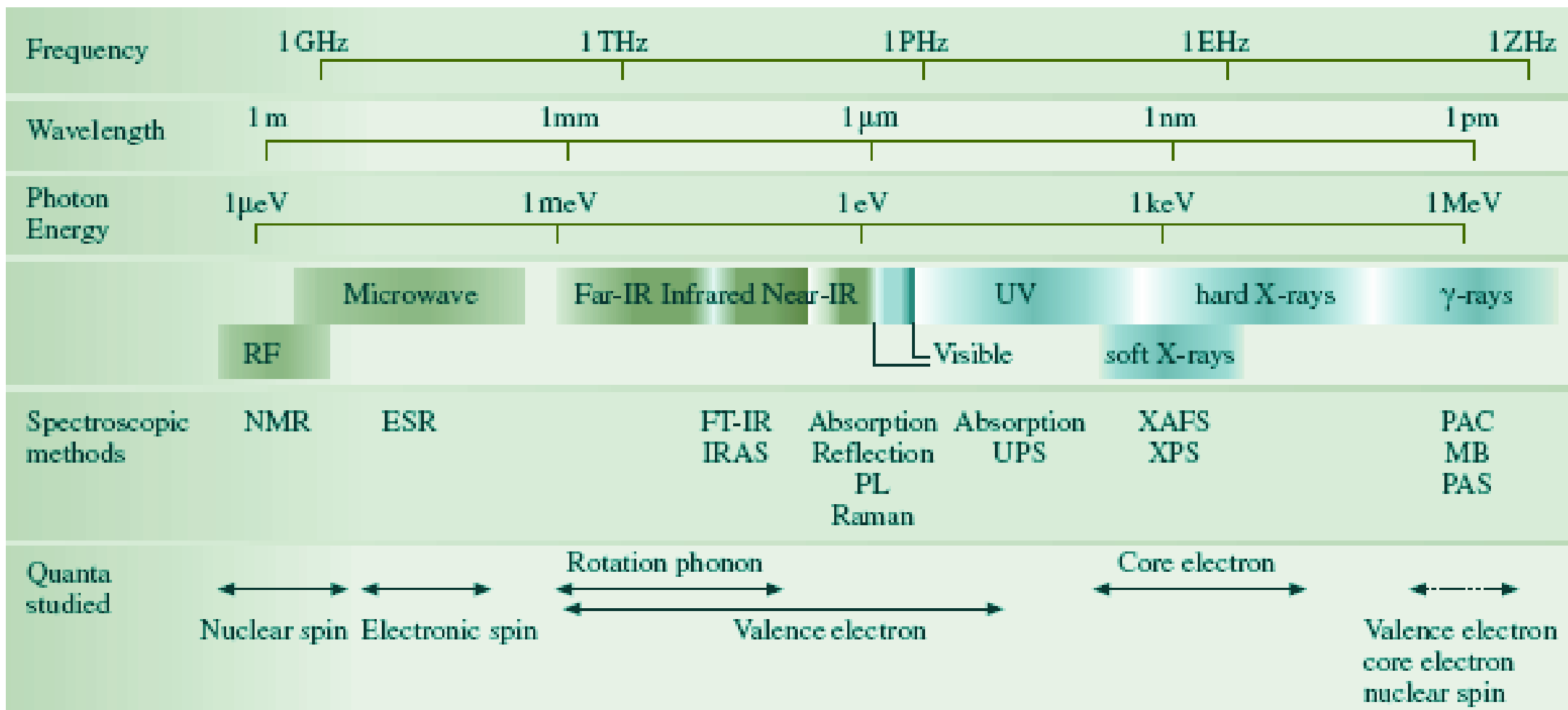


Instrumentations using radiation for material analysis need to be optimized :

- source characteristics
- detection characteristics
- sample environment
- mechanical design

# Interaction wave-matter

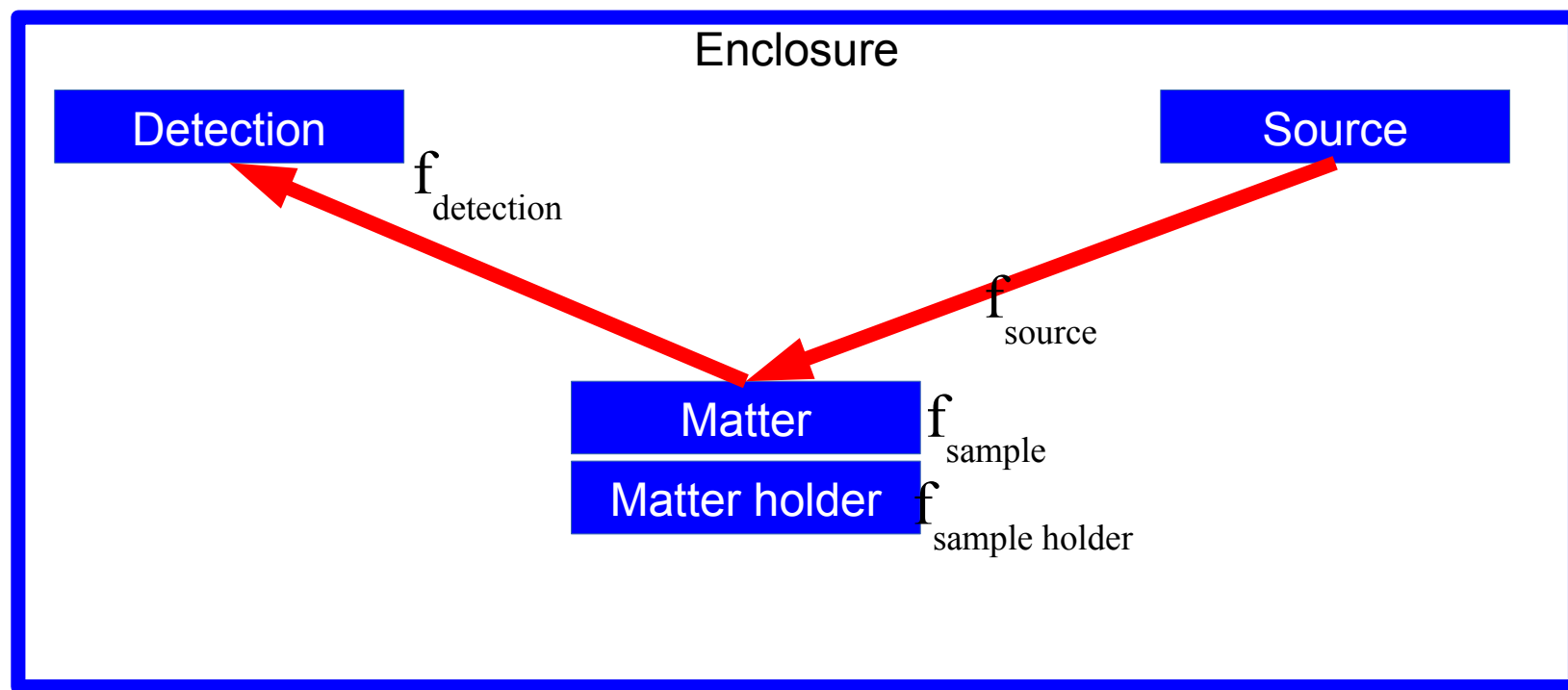
The energy of photons used for optical spectroscopic measurements of various quanta



EHz : exahertz ( $10^{18}$ ) - ZHz : zettahertz ( $10^{21}$ ) - YHz : yottahertz ( $10^{24}$ )

**Instrument is designed  
for the need  
we are looking for !**

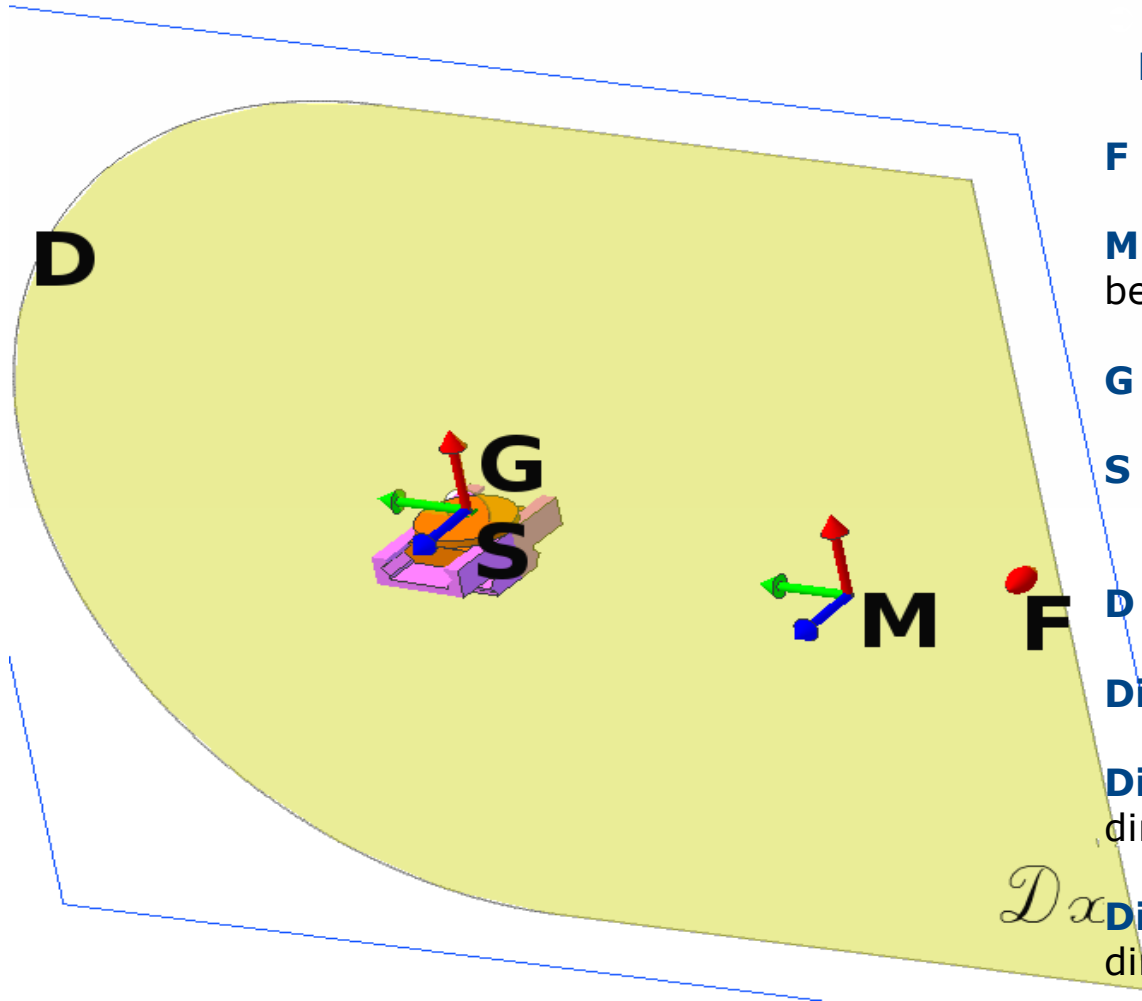
Instrument using a wave for probing matter is defined by several functions :



$f_{\text{operator}}$

Most instruments using radiation corresponds to this scheme :  
**XRD – XRF- FTIR- Raman-UV ...**

# Building an instrument: definition



**Dx** : Diffraction plane

**F** : focus of the source

**M**: Optical position (monochromator, mirror), involving a primary beam deviation

**G** : Goniometer center where is localized the sample

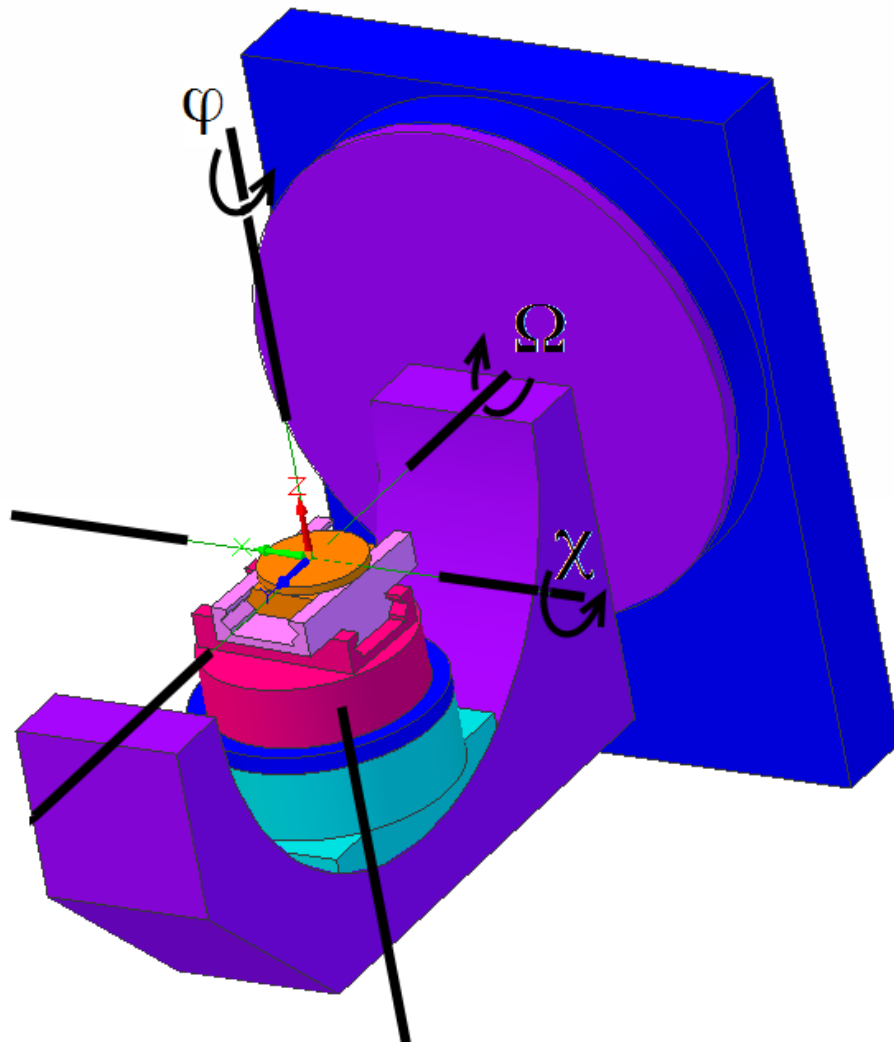
**S** : Sample position

**D** : Diffraction device

**Dir X**: Direction of the primary beam

**Dir Y**: Direction perpendicular to the diffraction plane (axial direction)

**Dir Z**: Direction perpendicular to the sample surface (equatorial direction)



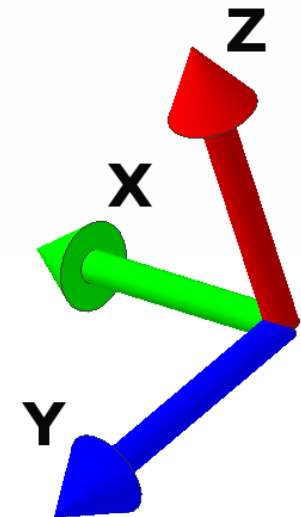
## Goniometer

Sample orientation is defined by 3 Eulerian angles:

- " $\Omega$ " angle is the incident angle on the sample surface
- " $\varphi$ " angle is the rotation belongs the normal axis to the sample surface
- " $\chi$ " angle allows to tilt sample belongs the axis intercept of the diffraction plane and sample surface

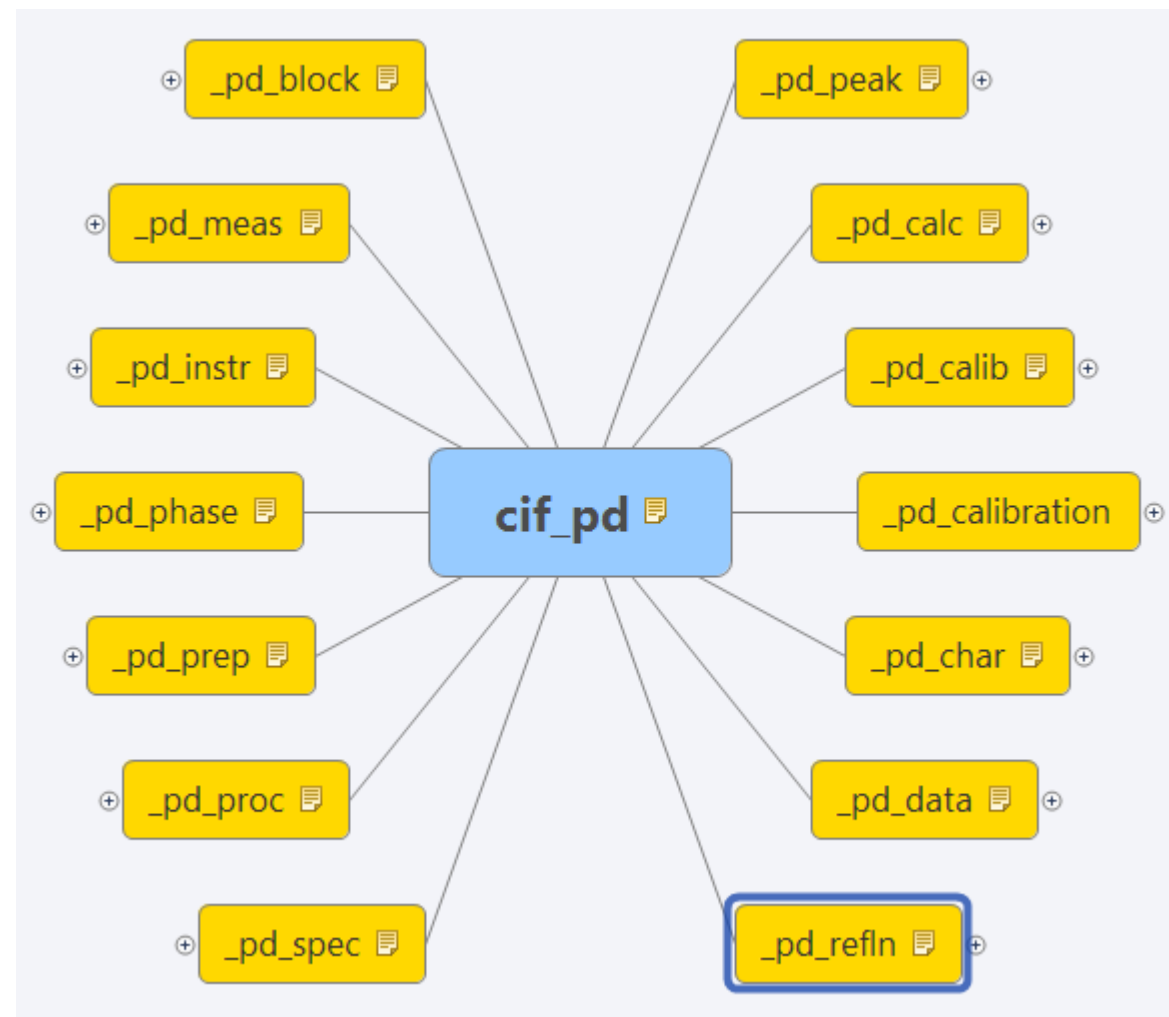
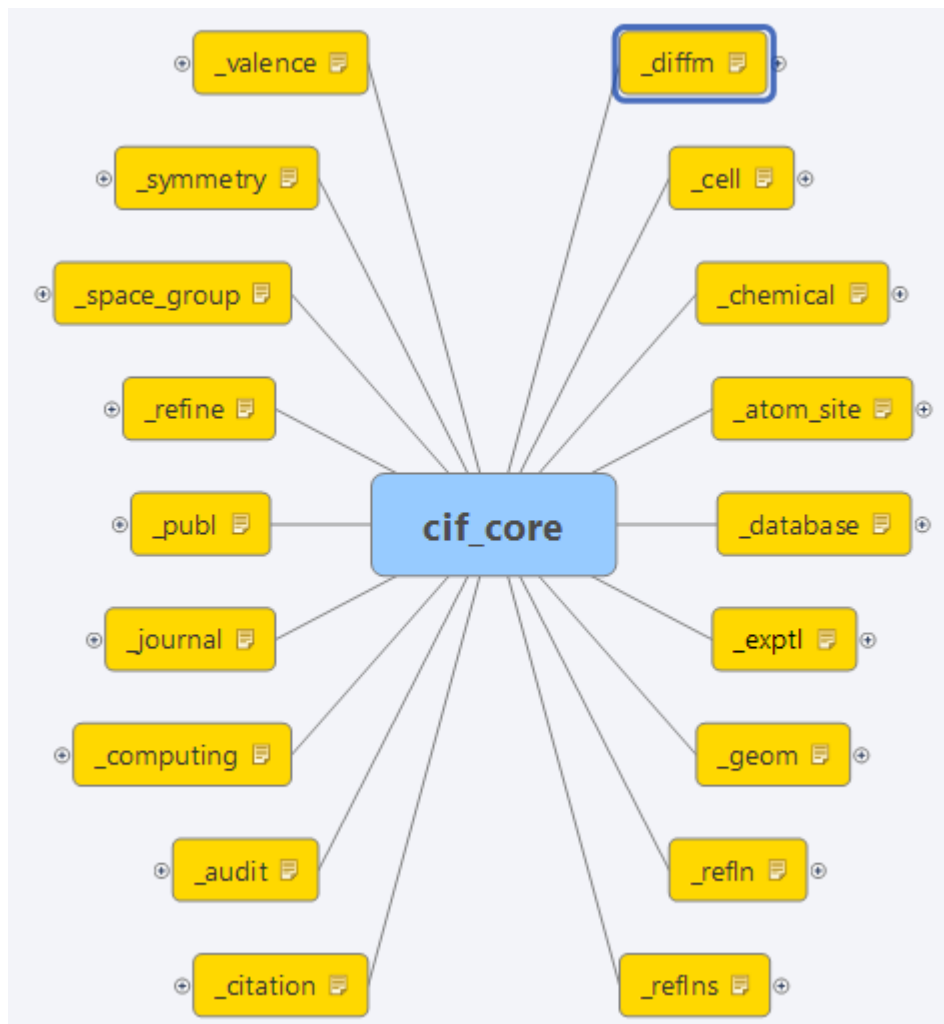
Remark:

- " $2\theta$ " angle belongs to the detection part



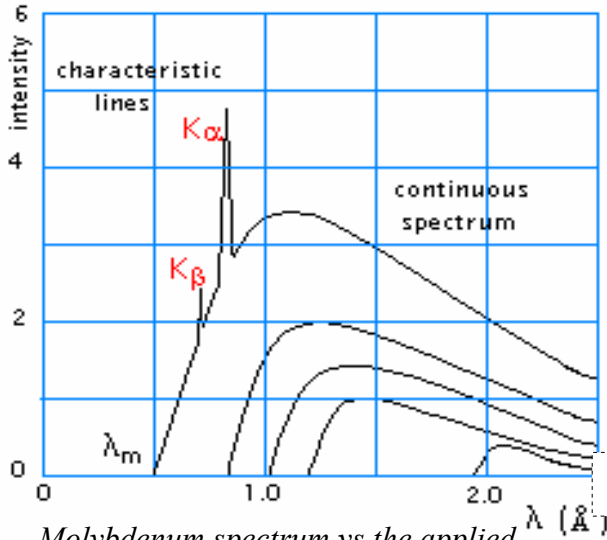
# A dictionary to describe the system: CIF

Defining and listing parameters make description easier !



[http://www.iucr.org/\\_\\_data/iucr/cifdic\\_html/1/cif\\_core.dic/index.html](http://www.iucr.org/__data/iucr/cifdic_html/1/cif_core.dic/index.html)

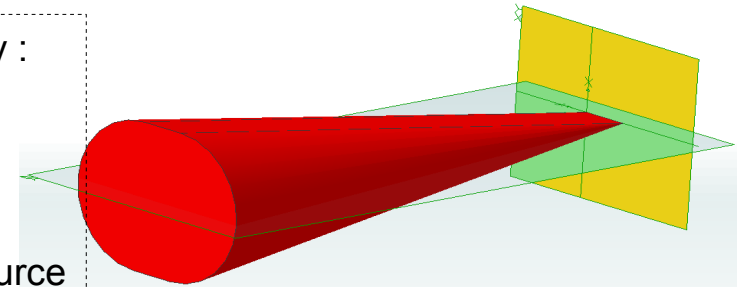
# Function source



Molybdenum spectrum vs the applied voltage

A light emission characterized by :

- a spectral range
- a solid angle
- intensity
- dimension and shape of the source



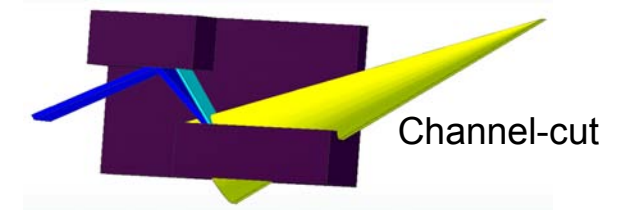
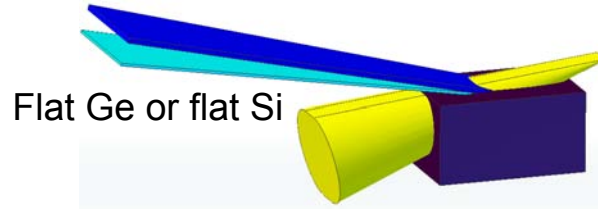
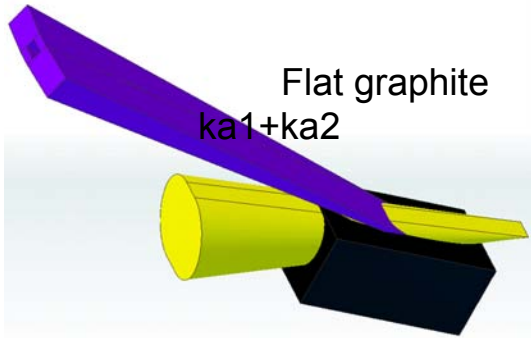
Optimizing the characteristics of a source allows to focus on a given interaction

	fluorescence	imaging	diffraction	reflection	diffusion
Spectral range	large	large	Monochromatic (excepted Laue)	monochromatic	monochromatic
Solid angle	Few degrees	Large (60°)	Small to parallel or focusing	Very small	Very small or focusing
Source size	Small or large	Small for resolution improvement	small	small	small
Source shape	point/linear	point	Point or linear	linear	Point or linear

This is achieved by using appropriate optics (1D, 2D, monochromator, mirror, collimator, slits ...)



# Function source; shaping the beam !

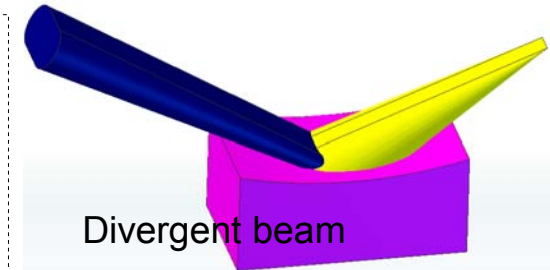
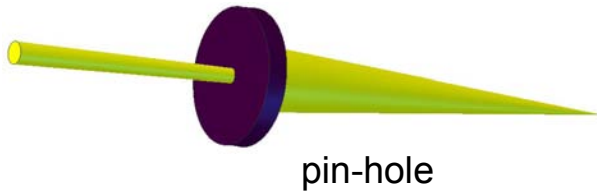


“Monochromaticity”

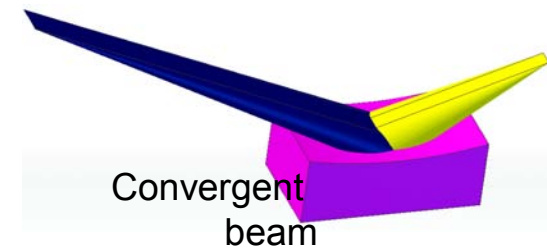
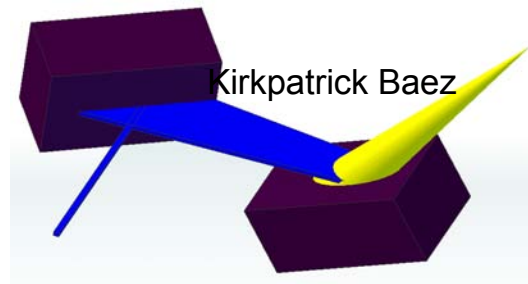
An optic is characterized by :

- mosaicity → spectral range
- a capture angle → beam size
- divergence → resolution

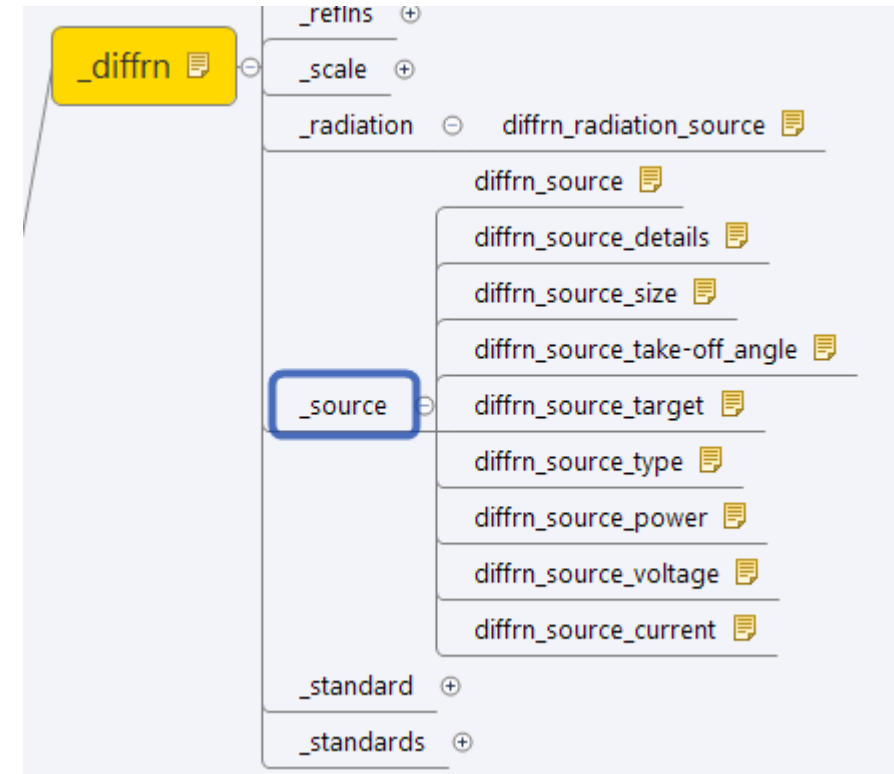
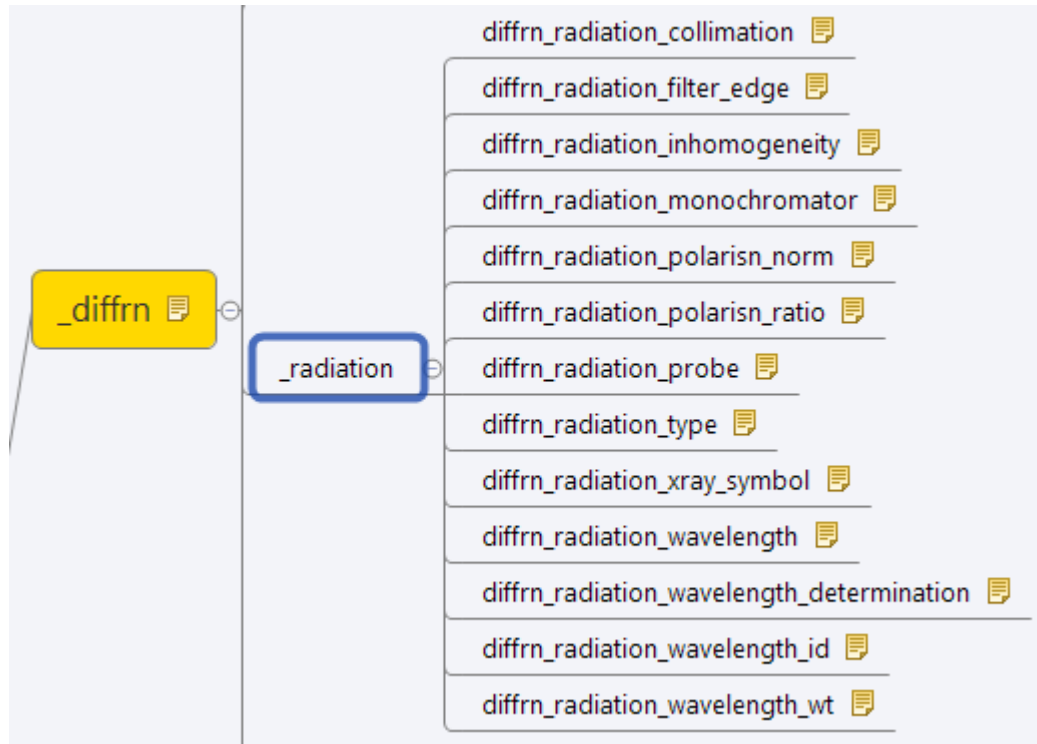
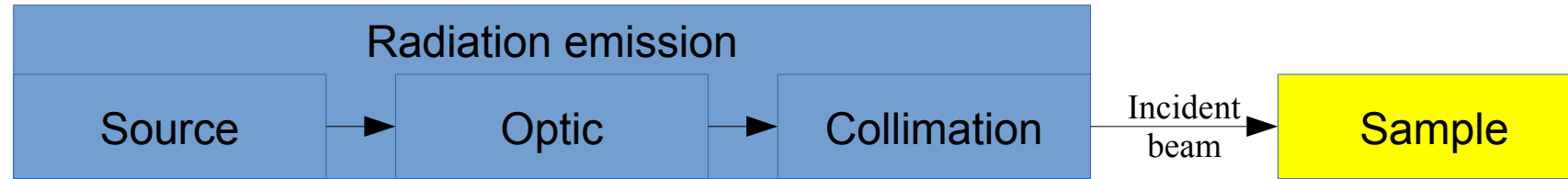
Divergence



Focusing



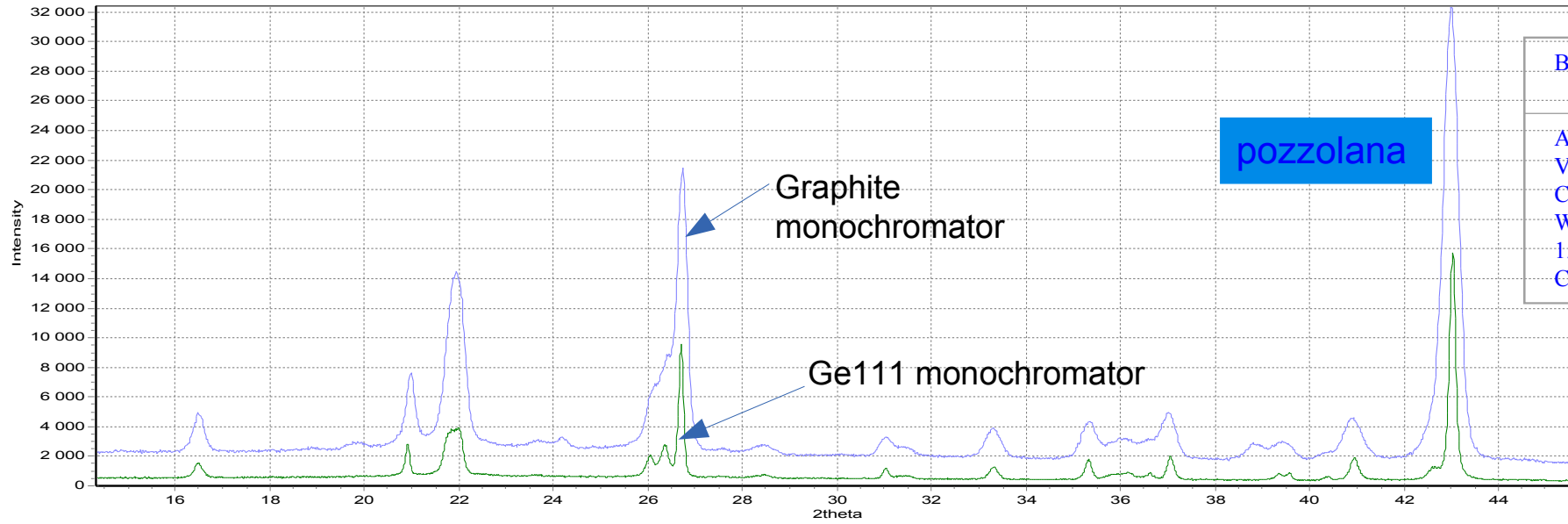
# A dictionary to describe the source



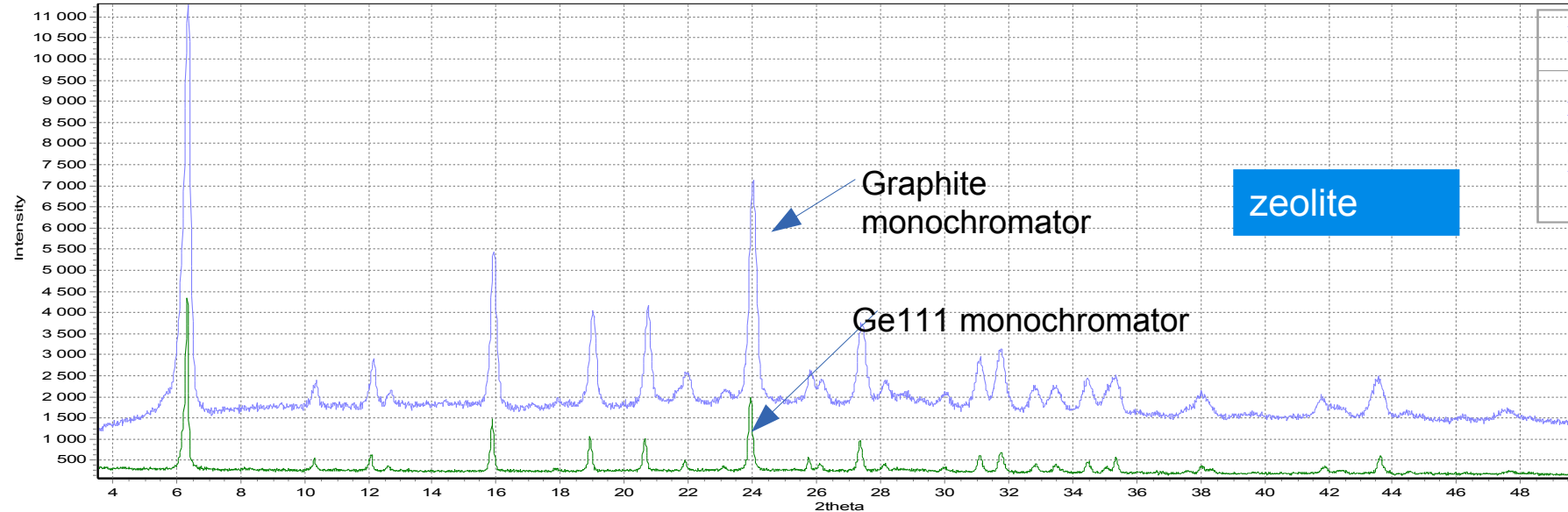
Deeper in the CIF !

Ones doing programming will see « object oriented programming »

# Effect of optic: comparison between high resolution and high flux

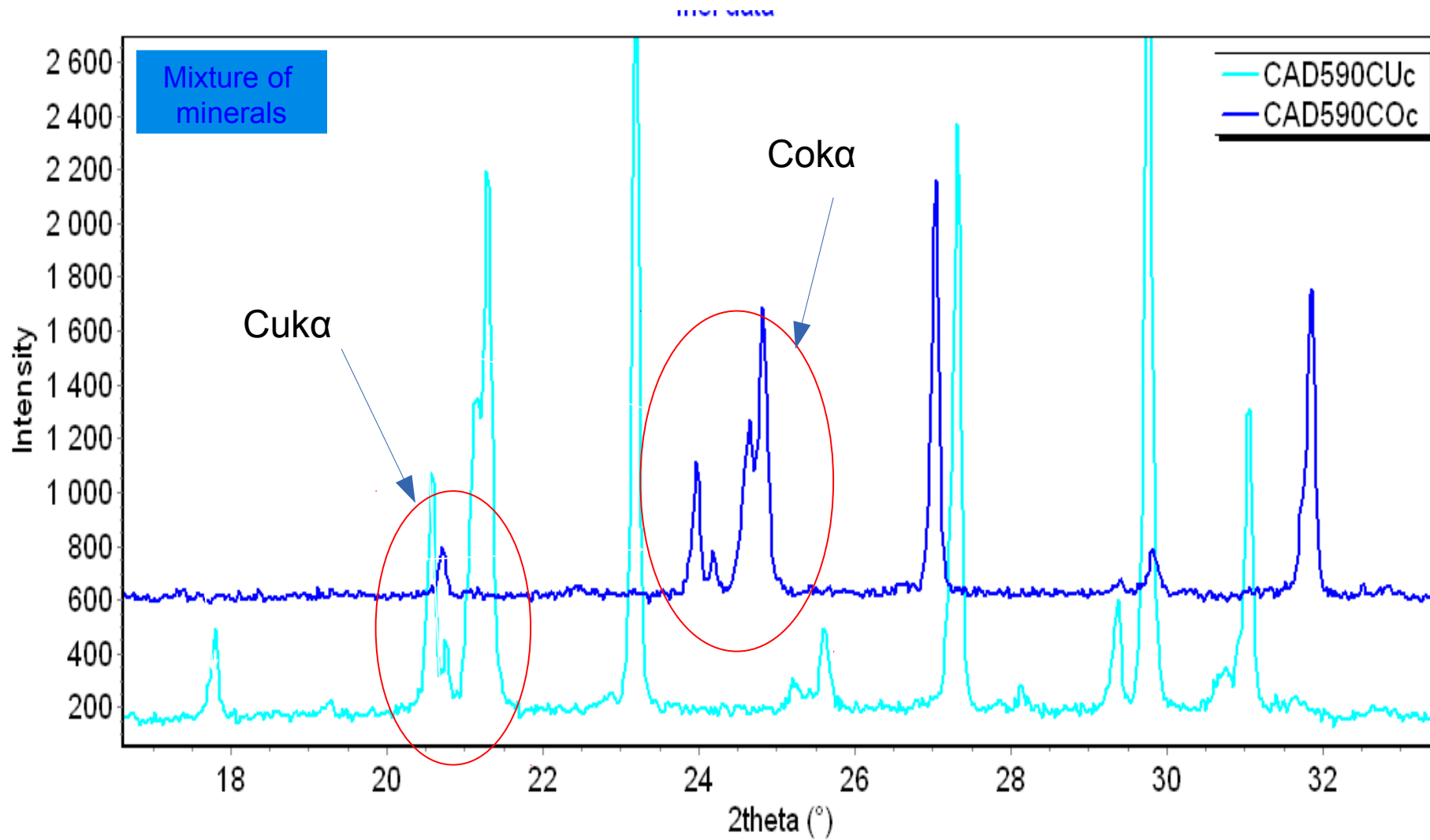


Blue	Green
ACQTIME 300	ACQTIME 27815
VOLTAGE 35	VOLTAGE 35
CURRENT 35	CURRENT 35
WAVELENGTH 1.5405600	WAVELENGTH 1.54056
COMMENT1 inc=10 SFspin	COMMENT1 inc=8 spin

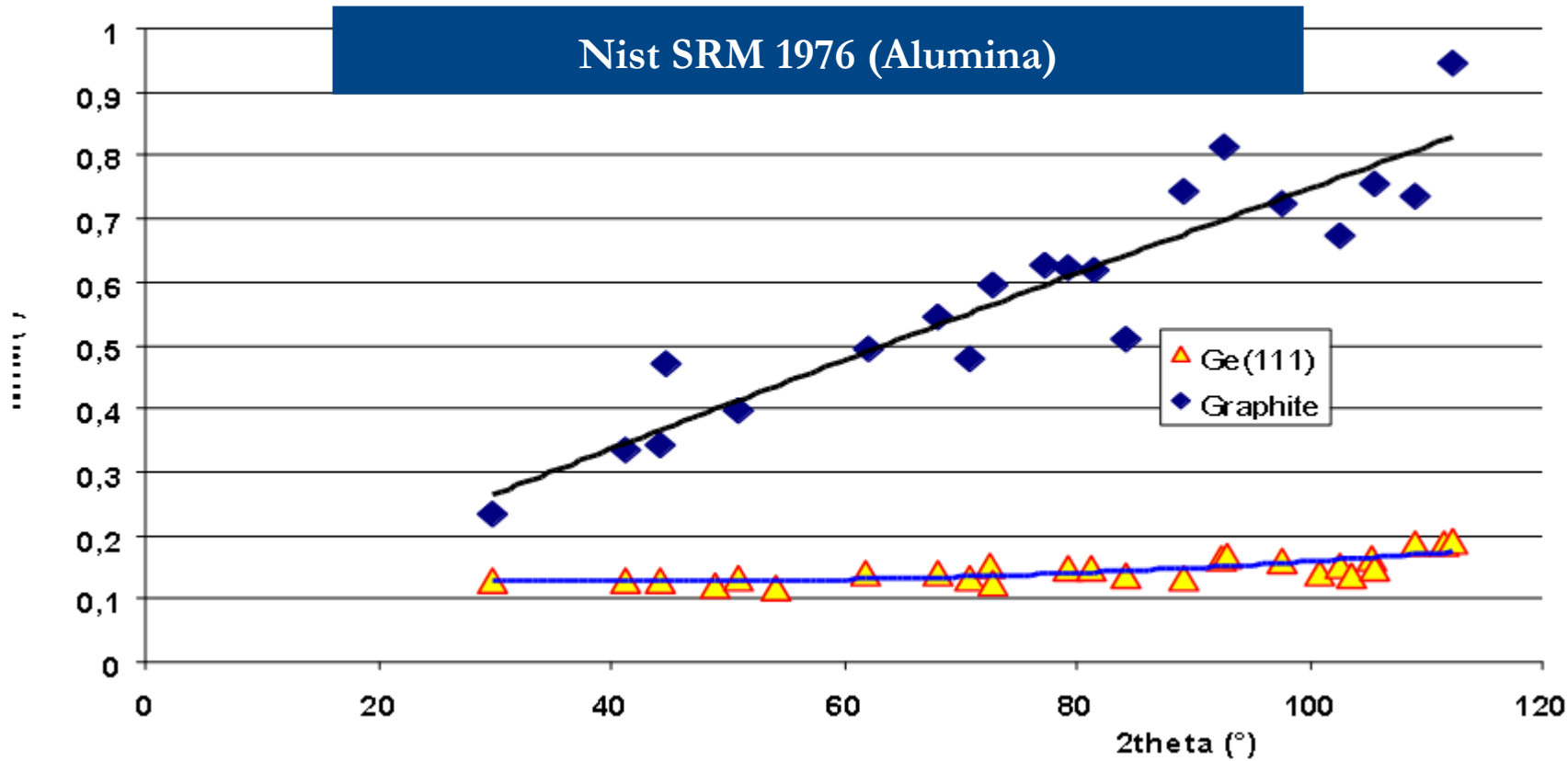


Blue	Green
ACQTIME 1800	ACQTIME 18000
VOLTAGE 35	VOLTAGE 35
CURRENT 35	CURRENT 35
WAVELENGTH 1.5405600	WAVELENGTH 1.54056

# Effect of wavelength



With graphite,  $ka_1/ka_2$  doublet is considered as a single peak.



	Flux ratio
Ge(111)	1
Graphite	5
parab. Mirror	15
Elliptical mirror	20

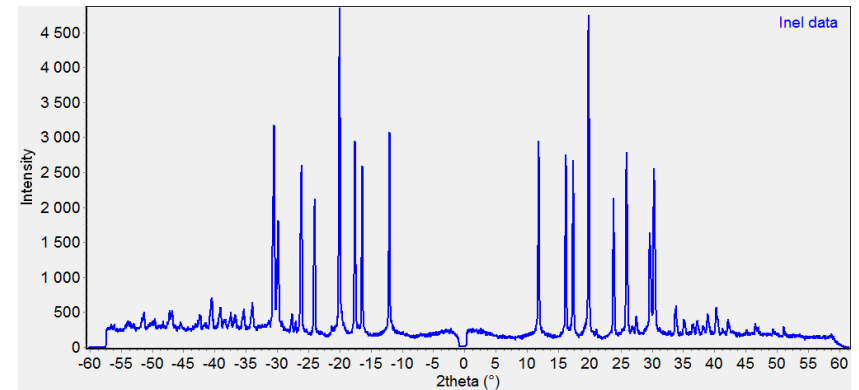
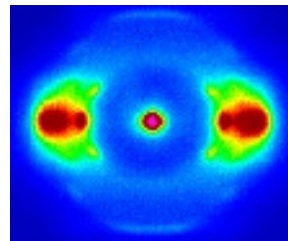
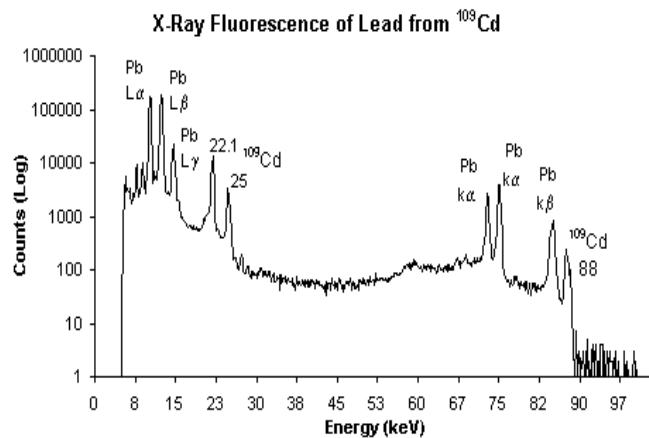
# Function detection

A detector is characterized by :

- spacial resolution
- dynamic range
- energy resolution
- dimension

Optimizing the characteristics of a detector allows to improve the measurement

	fluorescence	imaging	diffraction	reflection	diffusion
Spacial resolution	none	good	good	none	medium
Dynamic range	3	4~5	3~5	6~8	3~4
Energy resolution	~200eV	None Filtering possible	None or 1KeV	None or 1KeV	None or 1KeV
dimension	0D	2D (1D)	0D, 1D, (2D)	0D(1D)	1D-2D

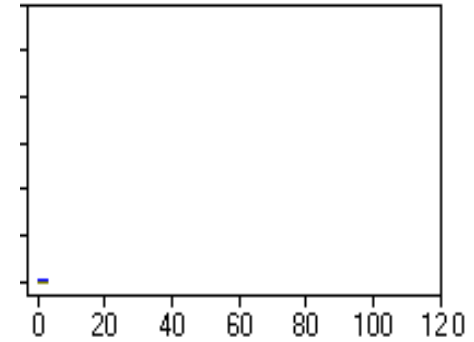
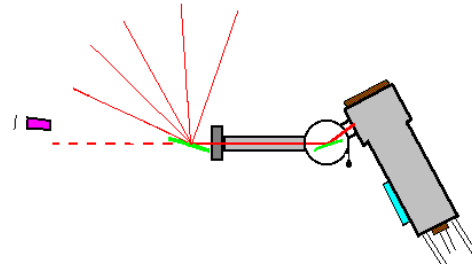


# Function detection

## 0D Detection :

Acquisition is done Stepwise

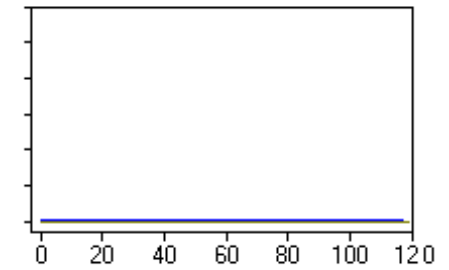
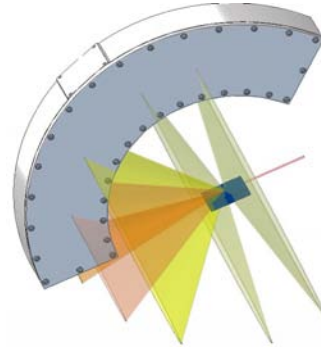
$2\theta$  and statistics are time dependent



## 1D Detection :

Acquisition is done in snapshots

Statistics is time dependent

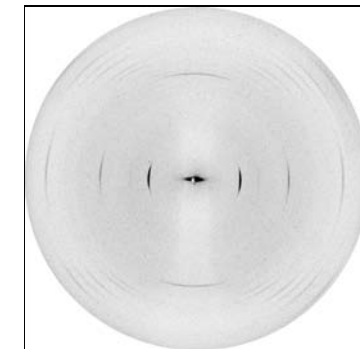
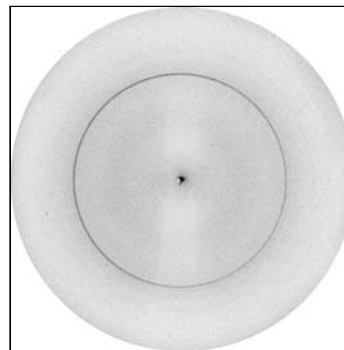


## 2D Detection :

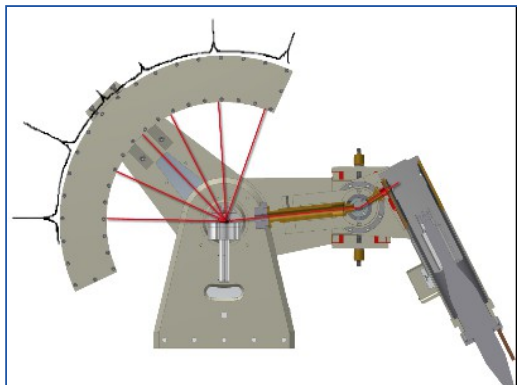
Acquisition is done in snapshots

Statistics is time dependent

Texture information but point beam required



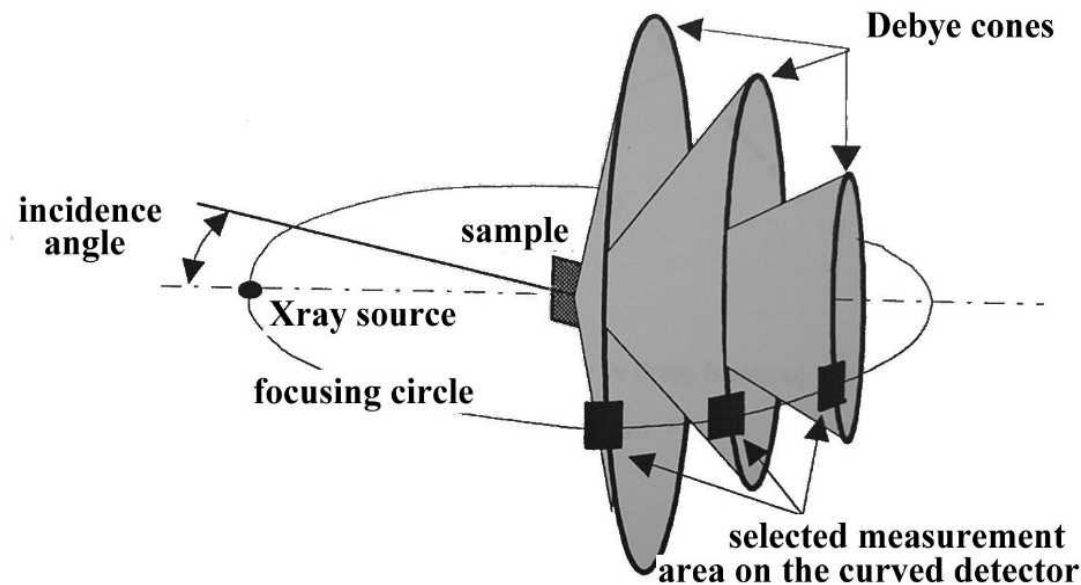
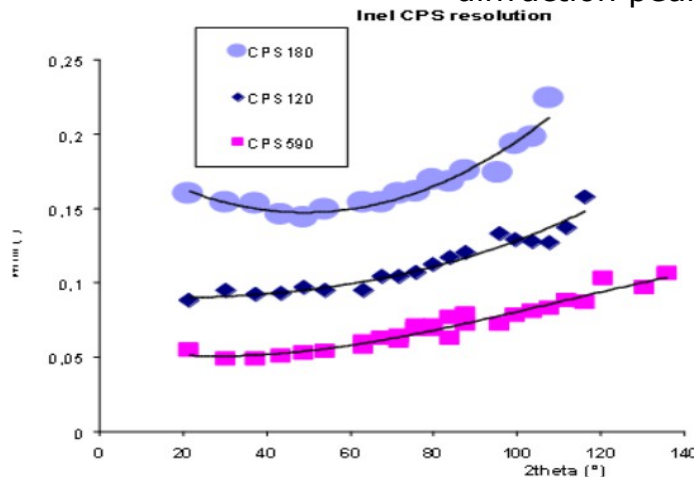
# A unique detection mode



## Curved detectors principle

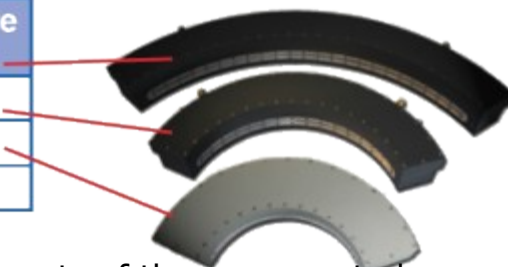
The EQUINOX diffractometers use the curved detectors principle, namely real time acquisition across a wide acquisition range.

- No motorization required: neither on sample nor on detector incidence
- Asymmetric acquisition mode: for a fix  $\theta$  sample incidence you can see all diffraction peaks on  $2\theta$  on the detector



## 3 detector types

	Detection angular range	Curvature (mm)
CPS 590	90° 2θ	R = 500
CPS 120	120° 2θ	R = 250
CPS 180	180° 2θ	R = 180

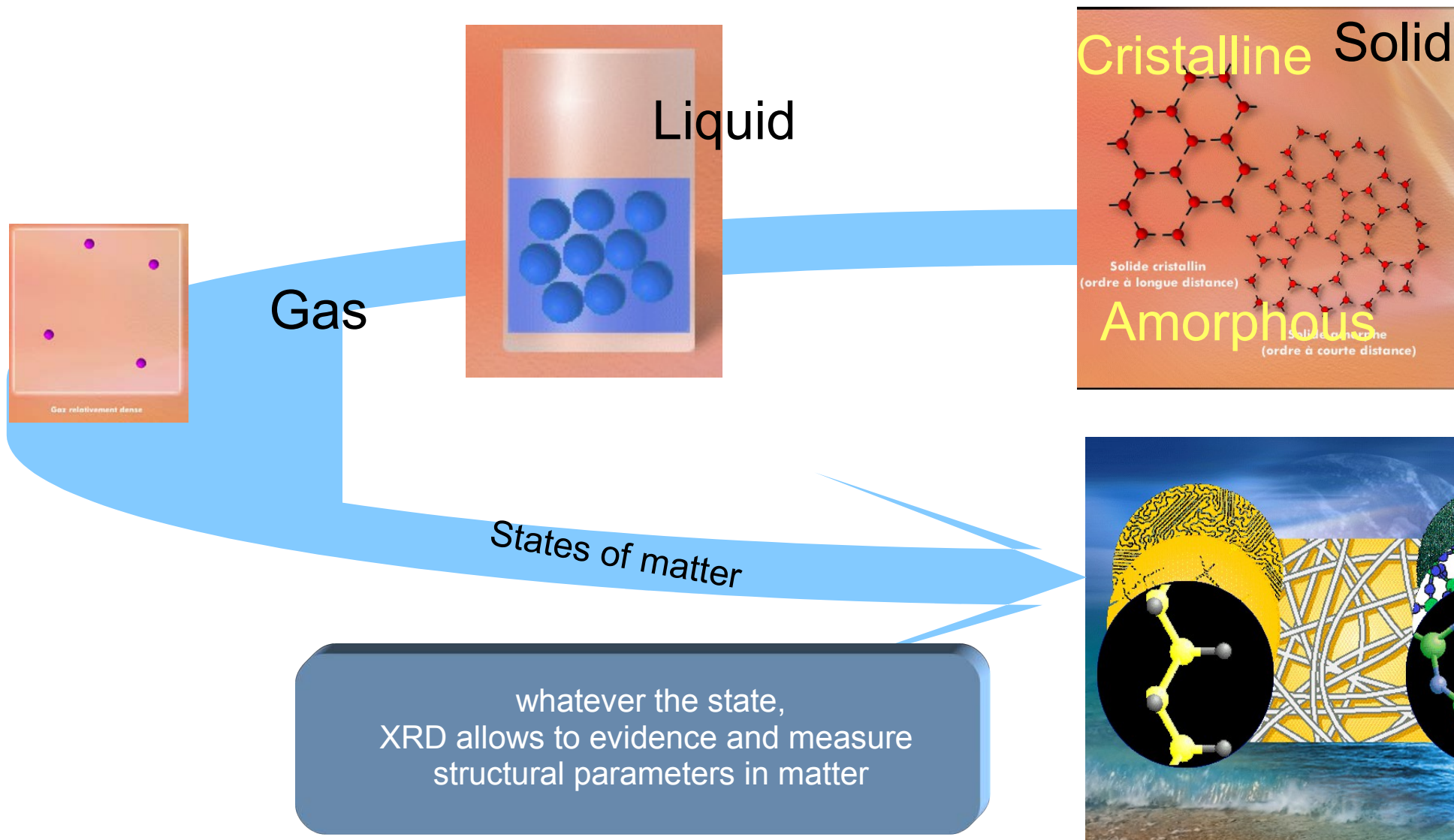


The detector choice depends on the requirements of the measure to be made:

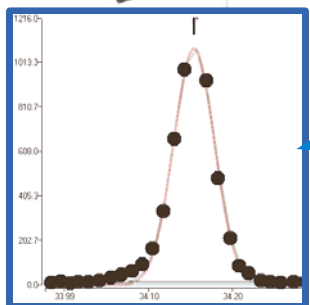
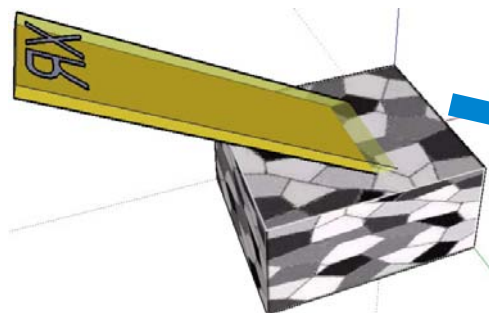
- The more the detector is far from the sample, the better the resolution will be
- The more the detector is near the sample, the faster the acquisition will be

**Analysis speed  
& resolution  
No maintenance**

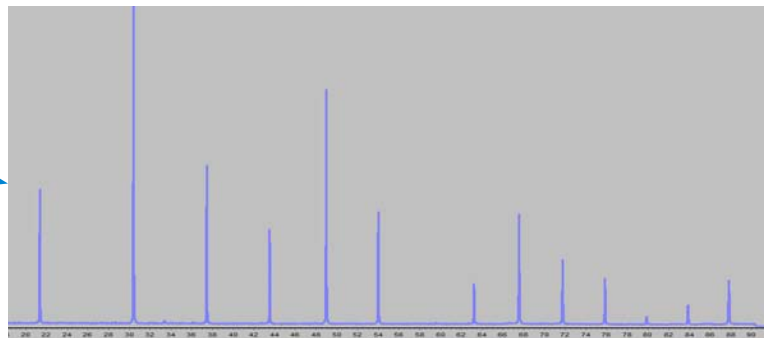




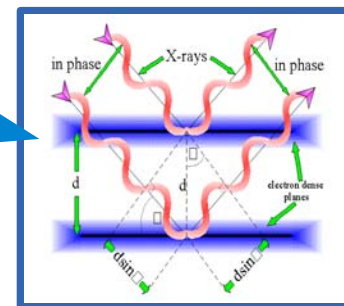
# Informations obtained by XRD



$$I = I_0 \cdot P \cdot L \cdot F^2 \cdot m \cdot A \cdot e^{-2M} \cdot \frac{1}{V^2}$$



Overall analysis of peaks shape, position and intensity and background function



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

What is the composition?  
and how much?

what is the crystallite size and morphology?

Is there any constrains inside crystallite?

Or in the overall sample?

Is there an organisation at the crystallite scale?

And can we quantify a distribution? Pole figures,

Structure, organization of electronic density levels :

What is the structural modification of my sample vs physical parameters (P, T...)?

Structural anisotropy :

Phase identification

Phases quantification

Particles size,

micro strains

Stress analysis

Preferred orientation (powder) or texture (bulk)

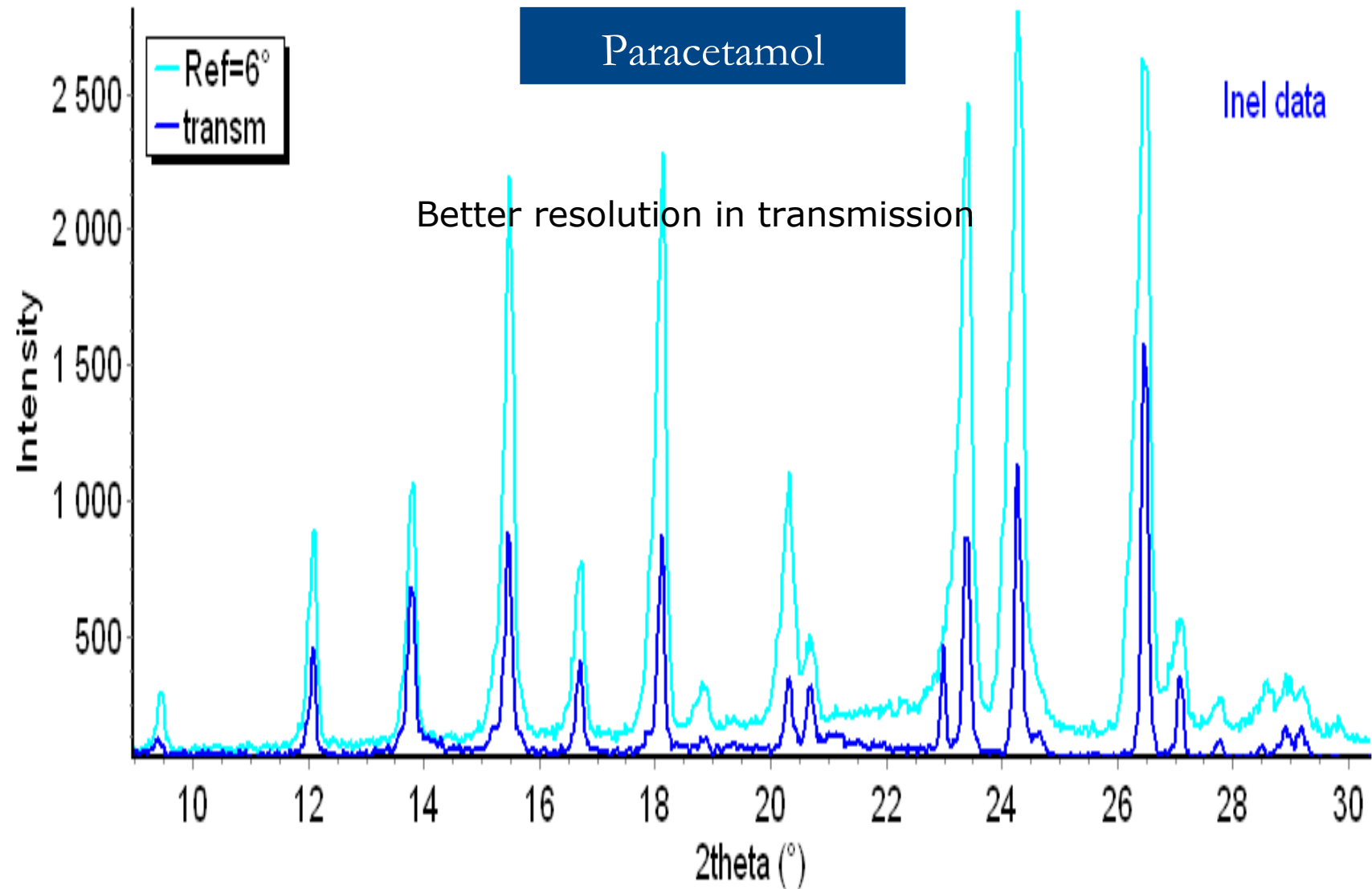
ODF

cell parameters, valence, atomic occupation, ...

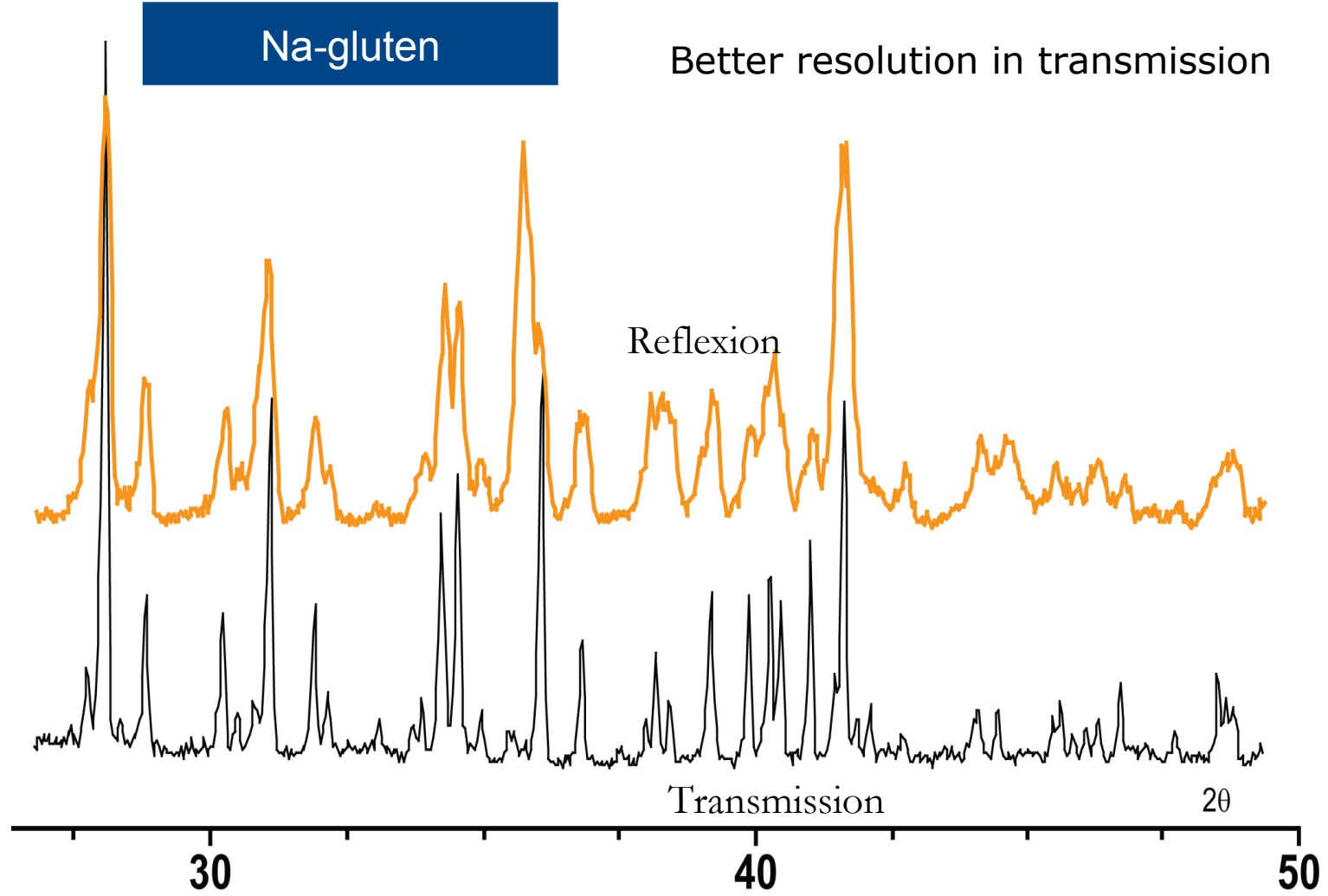
dilatation, phase transition

stress, texture, thin film characterization ...

# Function sample holder



# Function sample holder



## Understanding how to get the result

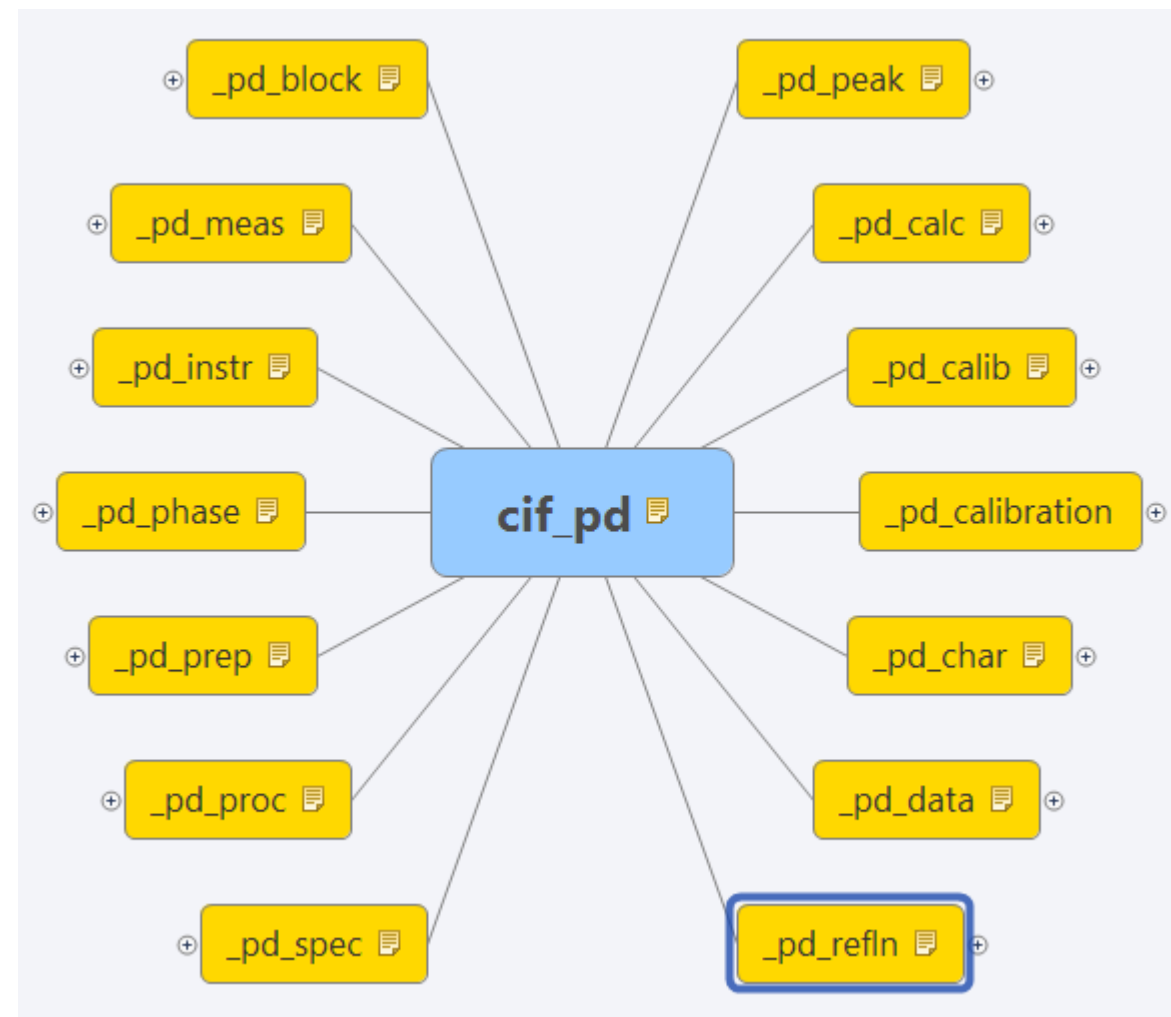
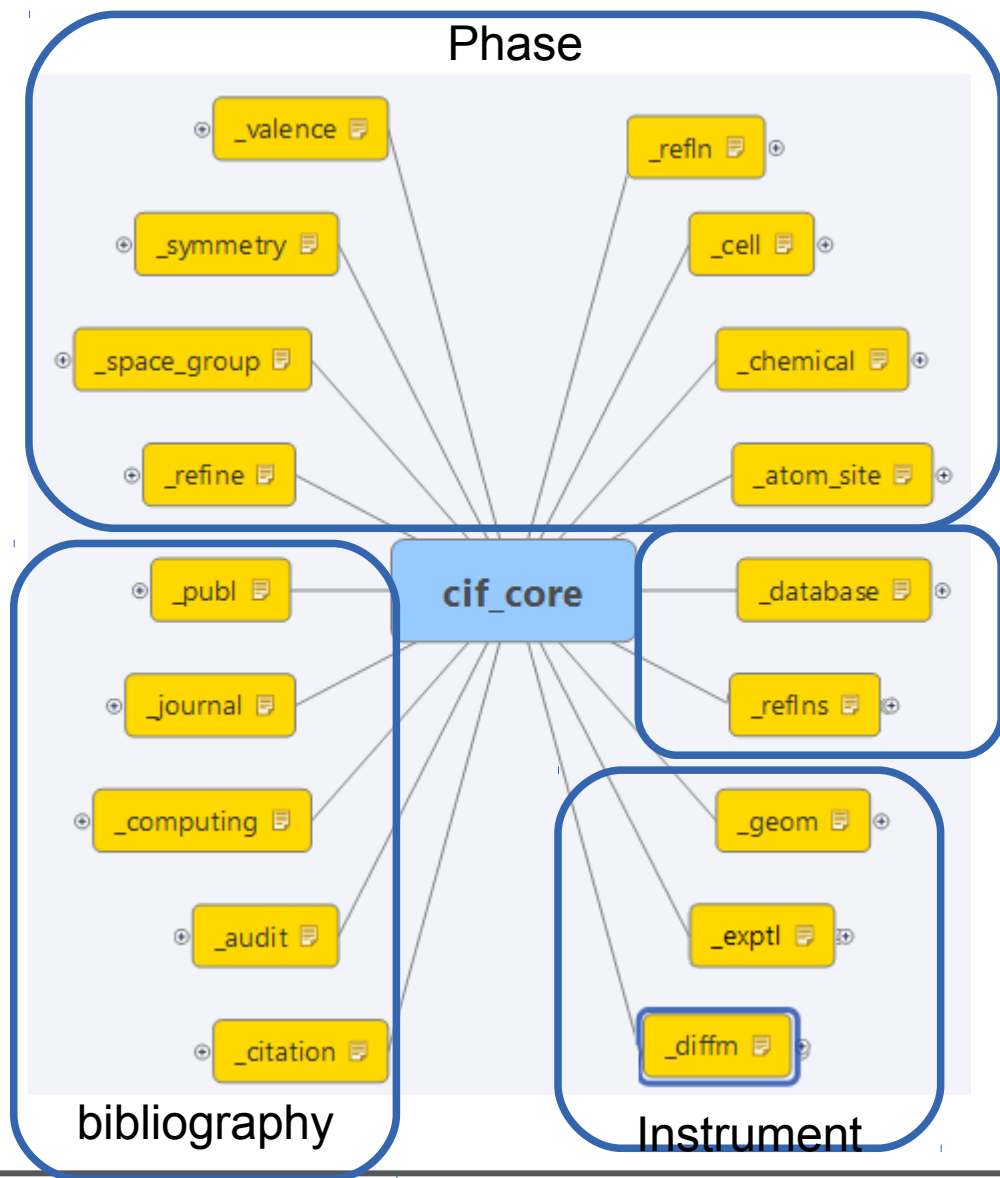
- appropriate instrumental configuration
- appropriate sample conditioning
- appropriate calibrations / corrections

		Type of solid	
		Single crystal	polycrystalline
Type of radiation	monochromatic	Rotating crystal Method	Powder XRD
	polychromatic	Laue Method	ED-XRD

## Some rules :

- Instrumental function is governed by all components of the XRD instrument :
  - source characteristics
  - optics and collimation
  - detection device
  - sample environment
- XRD components should be compatible to each other
  - Example : 1D optic is not recommended with a 2D detector (equatorial aberration)
- The good knowledge of the instrumental function allows to estimate as well the quality of the result
  - Example : absorption correction or LP correction are not the same in Bragg Brentano or in Debye Scherrer
- The instrument must be adapted to the requested measurement
  - Example : performing transmission measurement with Bragg-Brentano XRD is not appropriate
- Instrumental conditions must be correctly chosen (reproducibility of results)
  - Example : choose of the appropriate wavelength vs sample
- Use of appropriate standards
  - Example : in reflexion, eccentricity is influenced by transparency. Using standard with same absorption can correct this

# A dictionary to describe the system: CIF



# Existing Instruments And applications



# EQUINOX 100, stand alone benchtop XRD

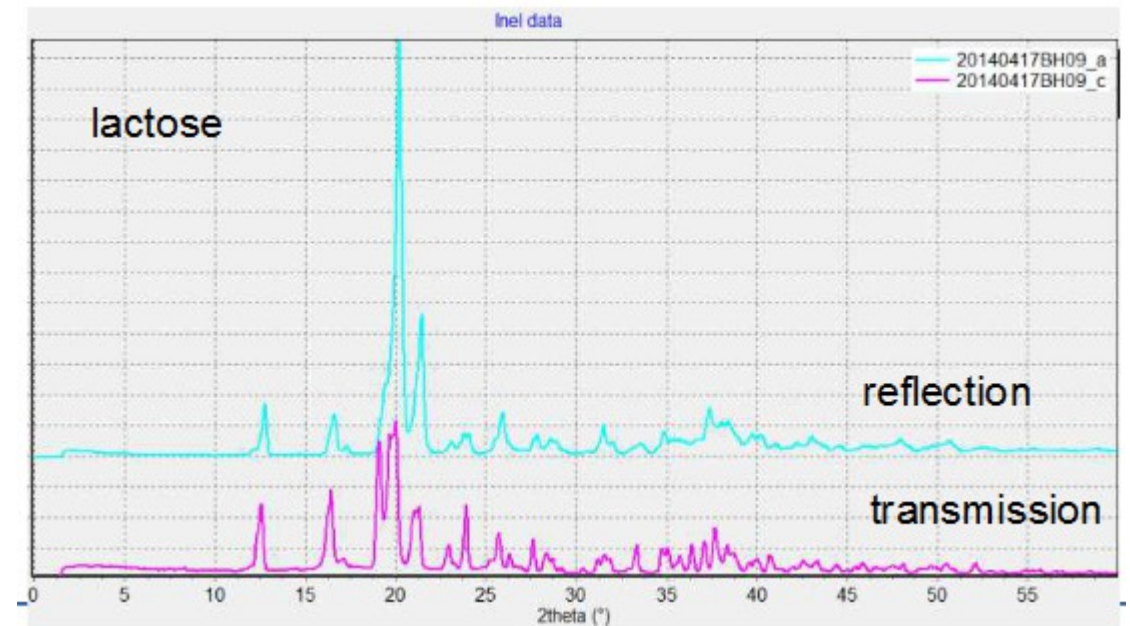
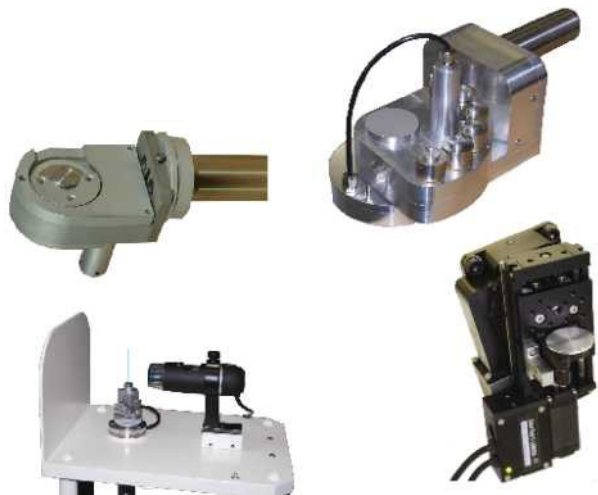


## A stand alone benchtop X-ray diffractometer

Designed for crystalline phases analysis (qualitative, quantitative, structural...) on powder or bulks. It is an ideal instrument for academic and QA/QC laboratories that need a small and easy to use equipment.

- Real time detection across  $110^\circ/2\theta$  (CPS180)
- Simplified goniometric deck with no motorization
- No external water cooling
- Works on standard power supply (110V-20A/230V-16A)
- Friendly-user instrument driving & data treatment software

**Applications:** qualitative & quantitative analysis, phases identification, structure determination, crystallites orientation...



# EQUINOX 1000, benchtop XRD



## A fast and powerful benchtop XRD

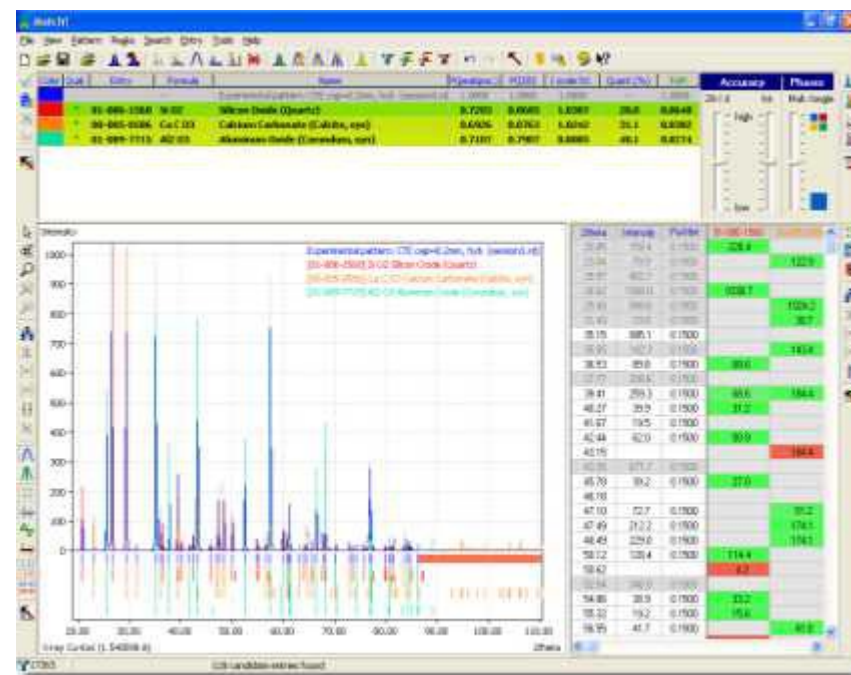
with small dimensions, ideal for all your X-ray diffraction applications on powder.

It is a very easy using instrument. No diffractometer alignment is required and the operating protocol is saved by the software. XRD experiments are available to anyone in a few moments.

- Real time detection across  $110^\circ/2\theta$  (CPS180)
- Monochromatic optics
- 3500 Watts generator
- External water cooling
- Working wavelength : Copper or Cobalt

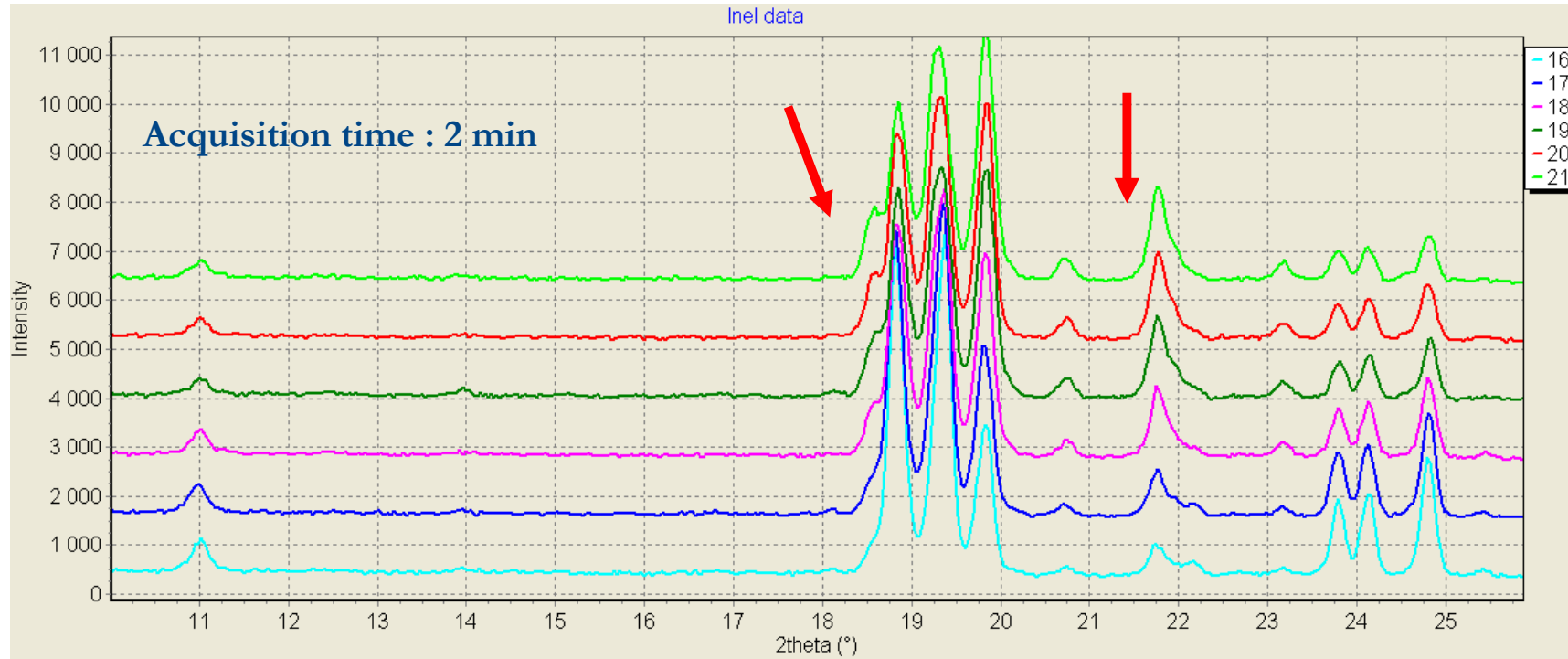
## Applications:

Qualitative & quantitative analysis, phases identification, structure determination, crystallites orientation...



# Quality control in detergent

On the graph below, are represented diffractograms recorded for each sample. We can clearly evidence an increase of STPP 1 with the index (red arrows).



Sample	16	17	18	19	20	21
STPP I	17,67%	25,9%	40,9%	51,35%	51,17%	60,2%
STPP II	82,33%	70,7%	56,93%	45,23%	46,57%	37,93%
Other	0,0%	3,3%	2,17%	3,43%	2,27%	1,87%

Quantitative analysis has been performed by using the **Rietveld** method. Good reproducibility, and good agreement with other techniques (chemistry)



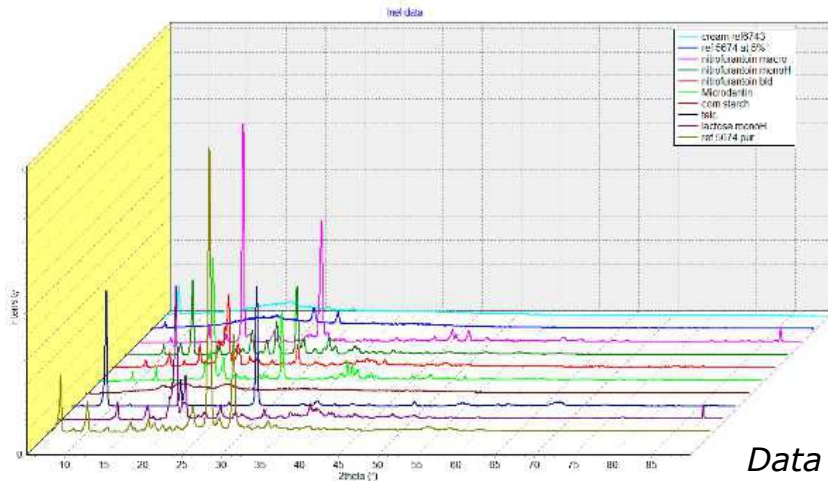
## A routine diffractometer

with the EQUINOX 1000 performances and a bigger sample space, the EQUINOX 2000 enlarges your applications capabilities. You can now realize variable temperature and/or atmosphere measurements.

- Fast results
- Thermodiffraction (phases transitions, unstable compounds)
- Large sample space
- Real time detection across  $110^\circ/2\theta$  (CPS180)
- Monochromatic optics
- 3500 Watts generator
- Working wavelength : Copper or Cobalt
- Environmental chambers (option)
- 30 positions auto-sampler (option)

## Applications

Qualitative & quantitative analysis, phases identification, structure determination, crystallites orientation, phases transitions under variable environments, ...



Data collection with sample changer

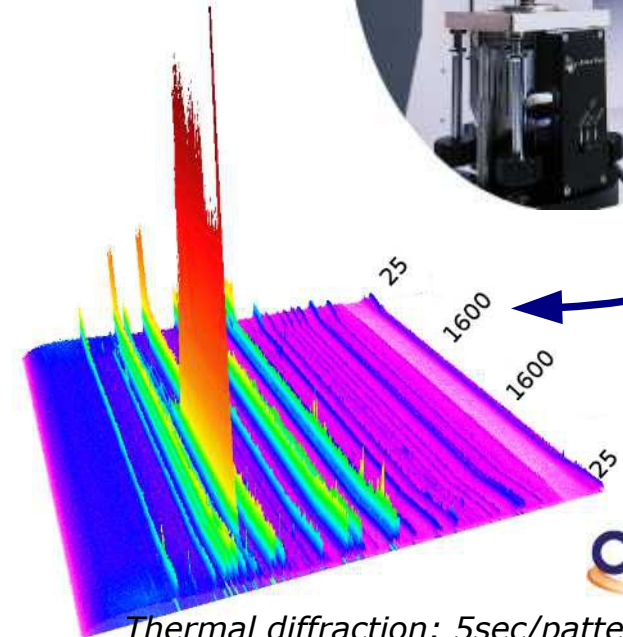
# EQUINOX 3000, powder high resolution XRD



## A fast, powerful and multi-purpose XRD

You are now able to realize variable temperature and/or atmosphere measurements, or even add a motorized sample holder to perform thin layer analysis.

- Evolutive depending on your needs
- Real time detection
  - CPS120 across  $120^\circ/2\theta$
  - CPS590 across  $90^\circ/2\theta$  (High resolution)
- Monochromatic optics
- 30 positions autosampler (option)
- Environmental chambers (option)



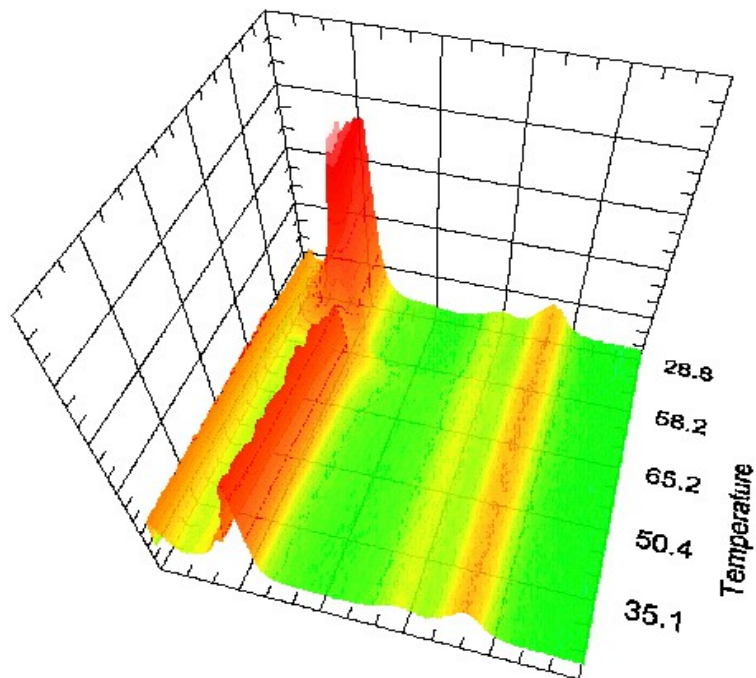
Thermal diffraction: 5sec/pattern

## Applications

Qualitative & quantitative analysis, phases identification, structure determination, crystallites orientation, phases transitions under variable environments, thin layer analysis, uniaxial stress analysis...

# Phase transition at low $2\theta$

Source : Copper  
Generator : 3,5 kW  
Optique : Parabolic mirror  
Incidence capillary) : Transmission (1mm  
Sample holder : non spinning  
furnace type FURCAP  
Detector : CPS120  
power : 35 kV – 35 mA  
Acquisition time : 3min  
setting : MPD



## Transition at 70°C

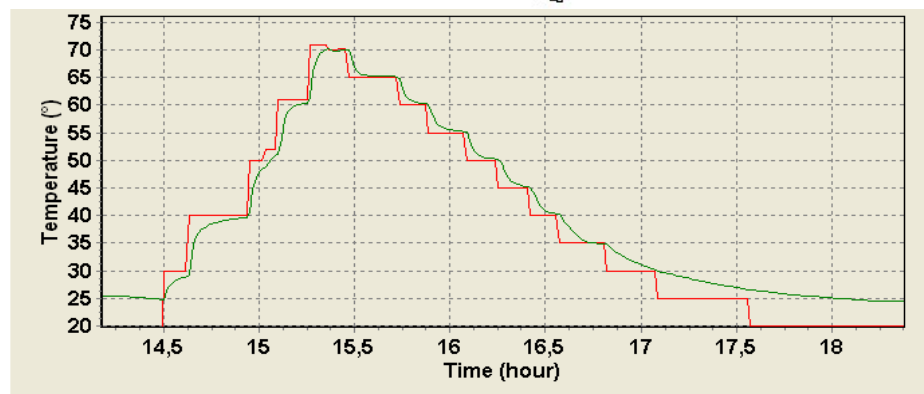
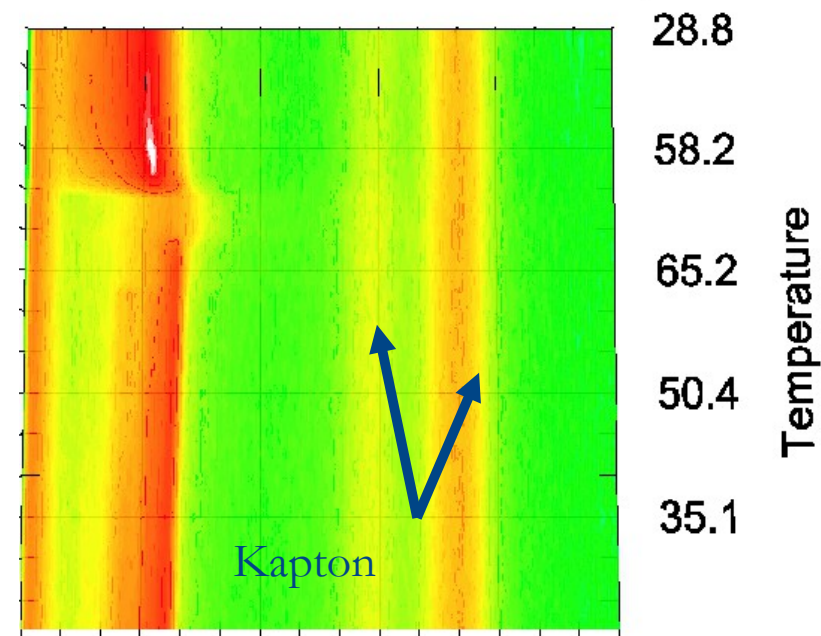
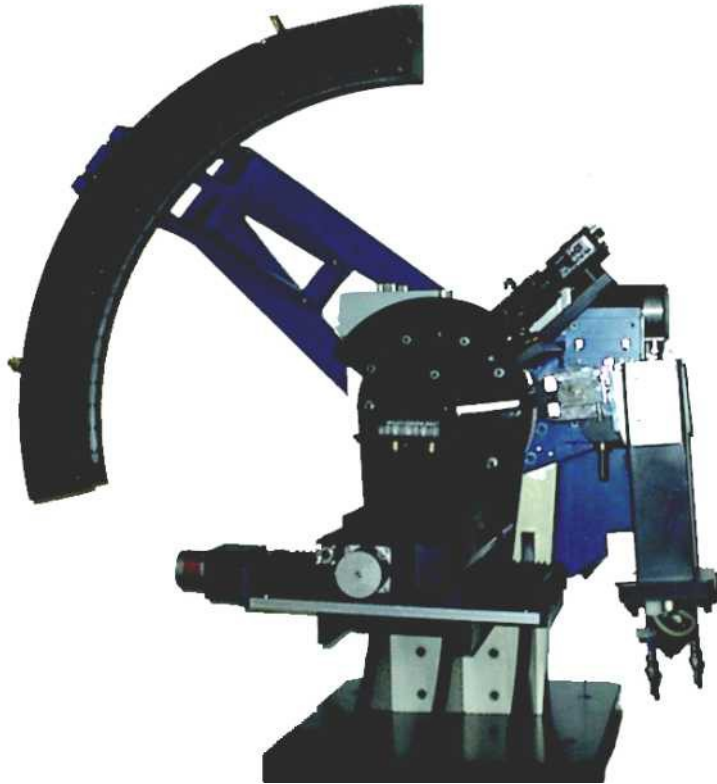


figure 1 : temperature profile : from RT to 70°C step 10°C and every 5°C while cooling down.

# EQUINOX 4000, DRX microdiffraction / cartographie

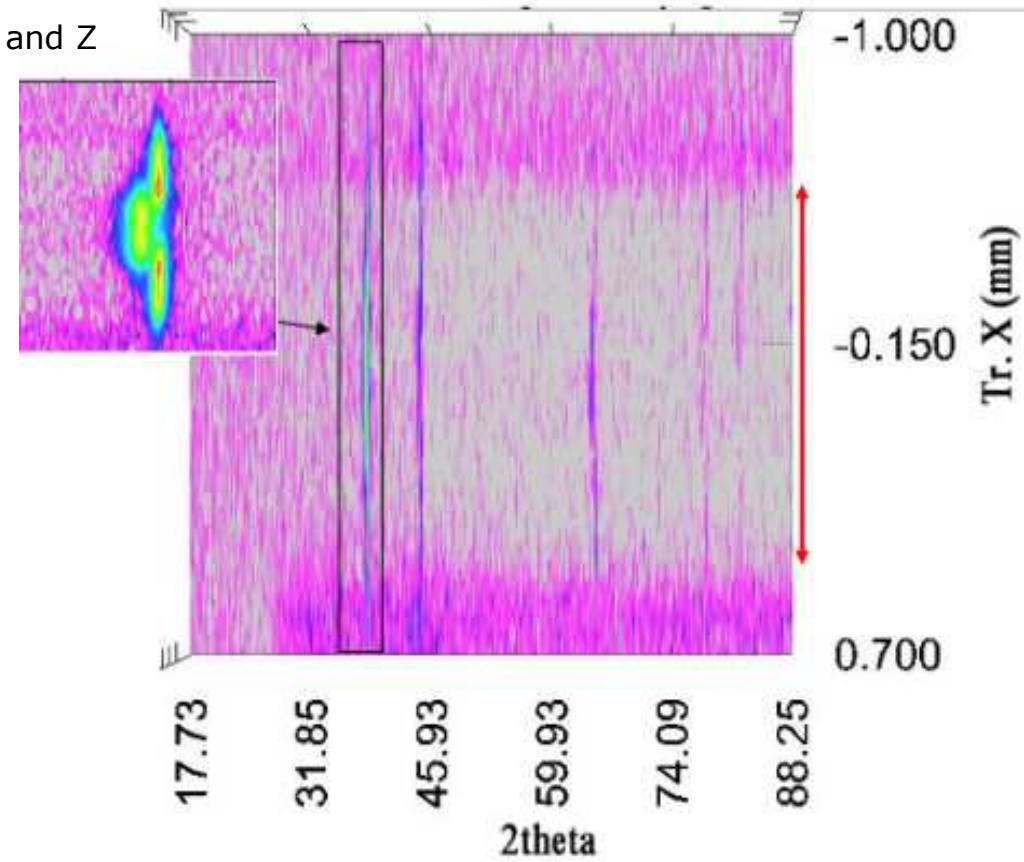
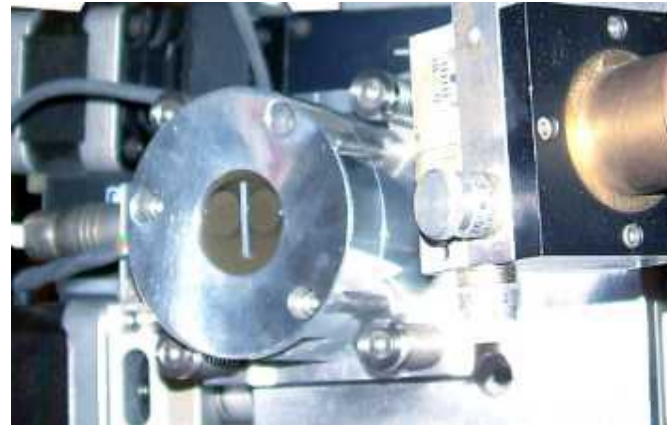


**EQUINOX 4000** is designed for all your microdiffraction or mapping applications. The instrument uses X, Y and Z translation stages with strong travel.

- Real time detector (CPS 120)
- $\theta / 2\theta$  goniometer with large stages X, Y and Z
- Working wavelength : Copper or Cobalt

## Applications

Microdiffraction, mapping...



*Microdiffraction on the edge of an aluminum plate*

Experimental: Beam size: 20mic, Power : 1200W  
Acquisition : 120sec/pattern

# EQUINOX 5000, high resolution XRD

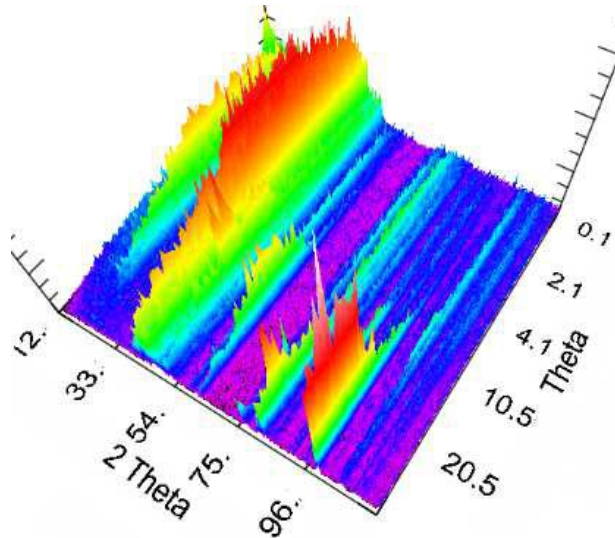
## A high resolution diffractometer

for all your powder analysis under variable temperature and/or atmosphere that require a very high resolution.

- $\theta/\theta$  or  $\theta/2\theta$  2 circles goniometer
- High resolution detection (CPS 590)
- Environmental chambers (option)

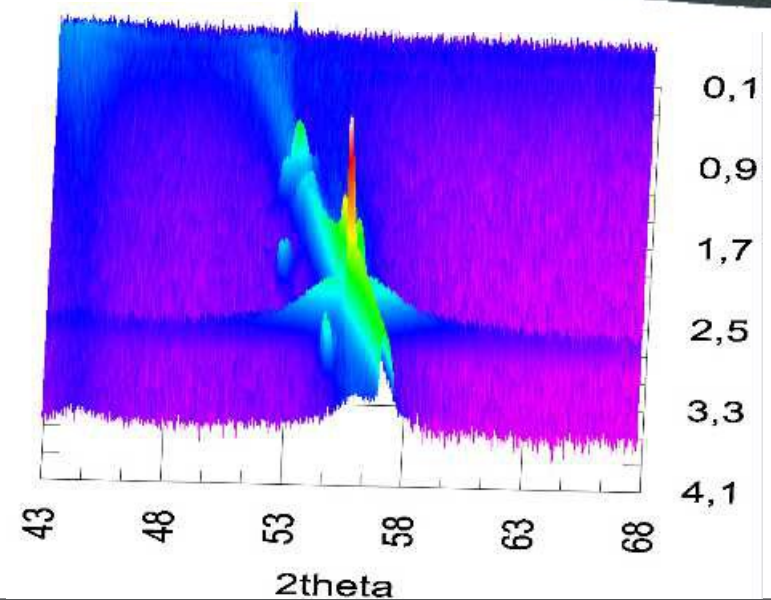
## Applications

Qualitative & quantitative analysis, phases identification, structure determination, crystallites orientation, phases transitions under variable environments, thin layer analysis, uniaxial stress analysis...



*Coating on stainless steel*

*Thin film analysis*





# EQUINOX 6000, 4 circles texture/stress XRD



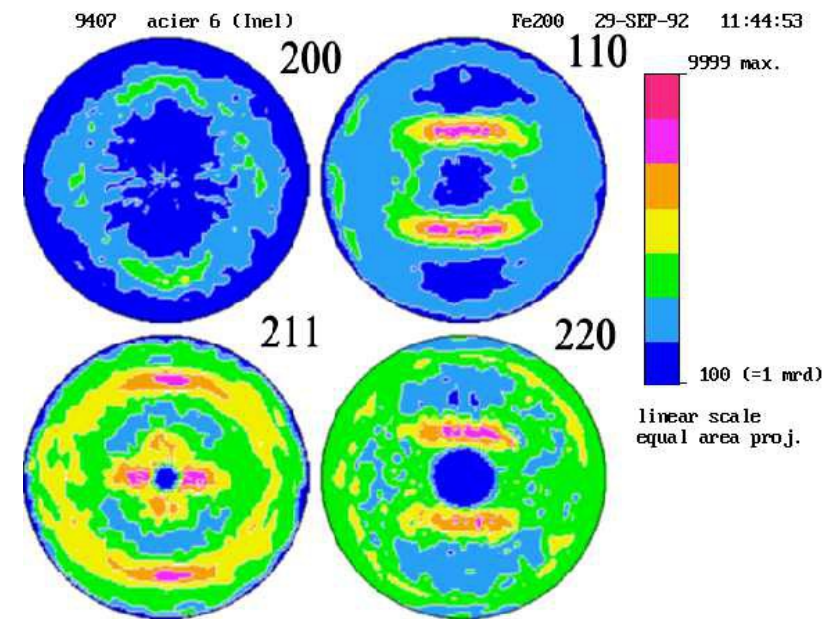
## 4 circles X-ray diffractometer

Ideal for all your 4 circles goniometer X-ray diffraction applications.

- Robust and multi-purpose goniometer
- Heavy loads accepted on every movements
- Large sample space
- Real time detection (CPS590)
- 4 circles goniometer ( $\theta$ ,  $2\theta$ ,  $\chi$ ,  $\phi$ )
- Collimating monochromatic optics
- 3500 Watts generator
- Variable working wavelength
- Temperature chambers (option)

## Applications

Texture, stress, thin layer, qualitative & quantitative analysis, phases identification, structure determination, crystallites orientation, phases transitions under variable environments, microdiffraction...



*Texture analysis on stainless steel foil*



- Evolutive mounting
- Variable sample/detector distance
- Specific supports and chambers available
- 1D or 2D detection with dedicated software

## Applications

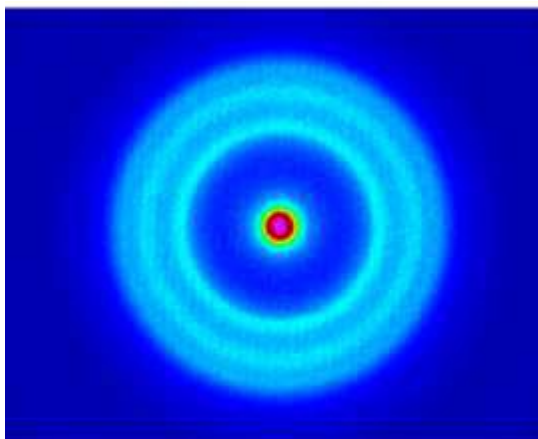
Colloids, metals, cement, clays, oil, polymer, plastics, proteins, pharmaceutical industry...

## Small Angles X-ray Scattering

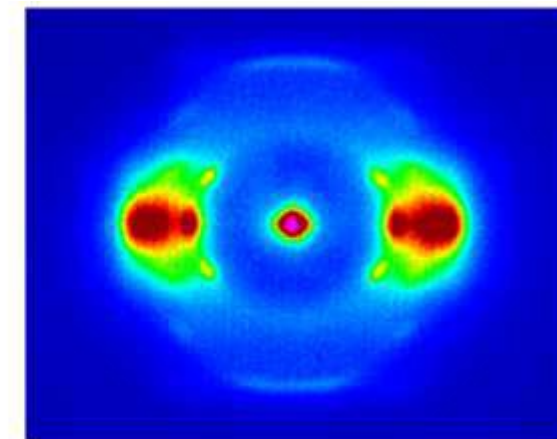
To better answer its customers needs, Inel designed a flexible SAXS line to make textured samples analysis or small angles scattering.

This technique is used to determine particles structure at nanometric range (size, form, distribution...). Studied materials can be solid, liquid or gas. This non-destructive method is accurate and requires usually only a minimal sample preparation.

It can be used as well for research as for QA/QC.



PET semicristallin (30%)



PET semicristallin (30%) déformation 1,4

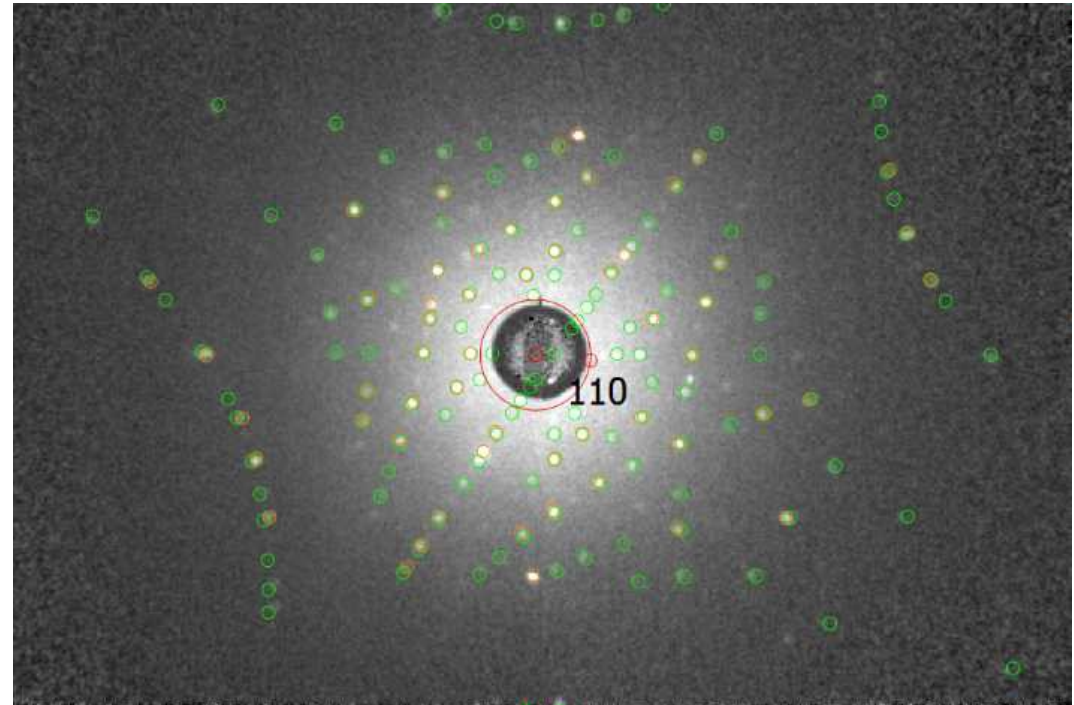
# Laue back reflection diffractometer



## A fast tool for cristal orientation

- Easy sample positioning
- Fast acquisition
- Fast orientation determination

Sample holder can be customized according to cristal



*Si220 orientation*

## Inel XRD flexibility

Combining X-ray diffraction with other techniques:

- One sample and several datas
- Real time analysis
- XRD comes to sample
- XRD for on line industrial control

## Inel portable XRD systems:

EQUIRAM

Combination of XRD and Raman spectrometer

XRD/DRIFT

Combination of XRD and DRIFT spectrometer

STRESS/WAXS

Combination of WAXS and stress analysis

SWAXS

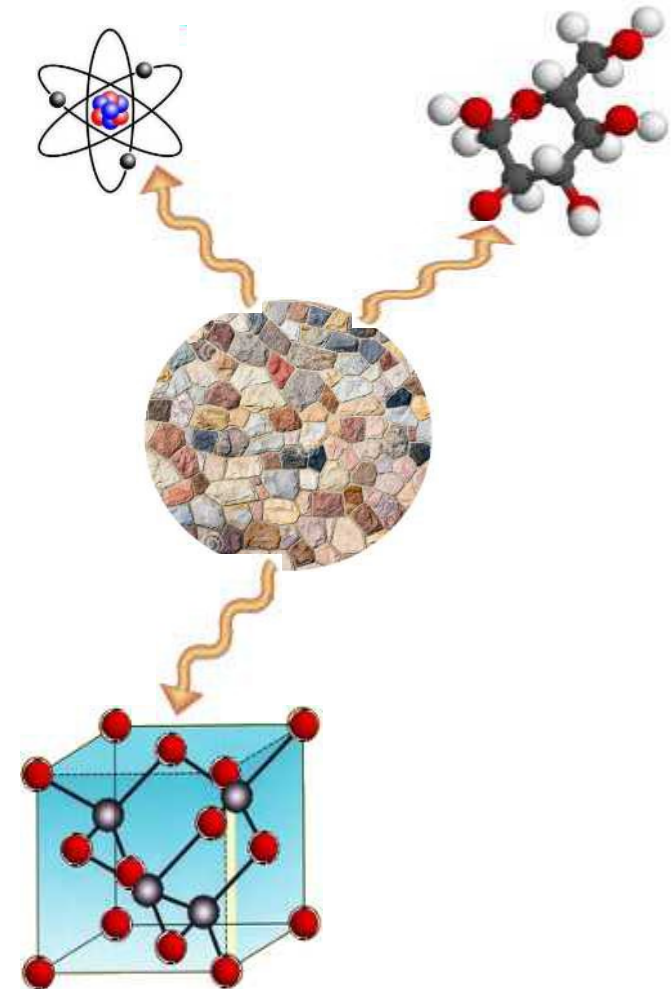
SAXS WAXS diffractometer

COSMA

On-line production control XRD

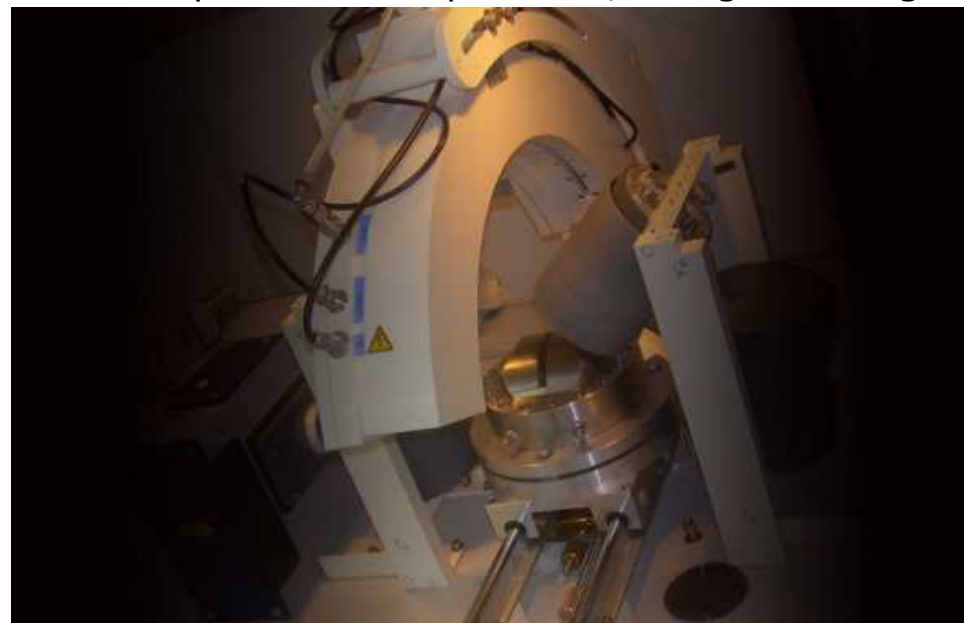
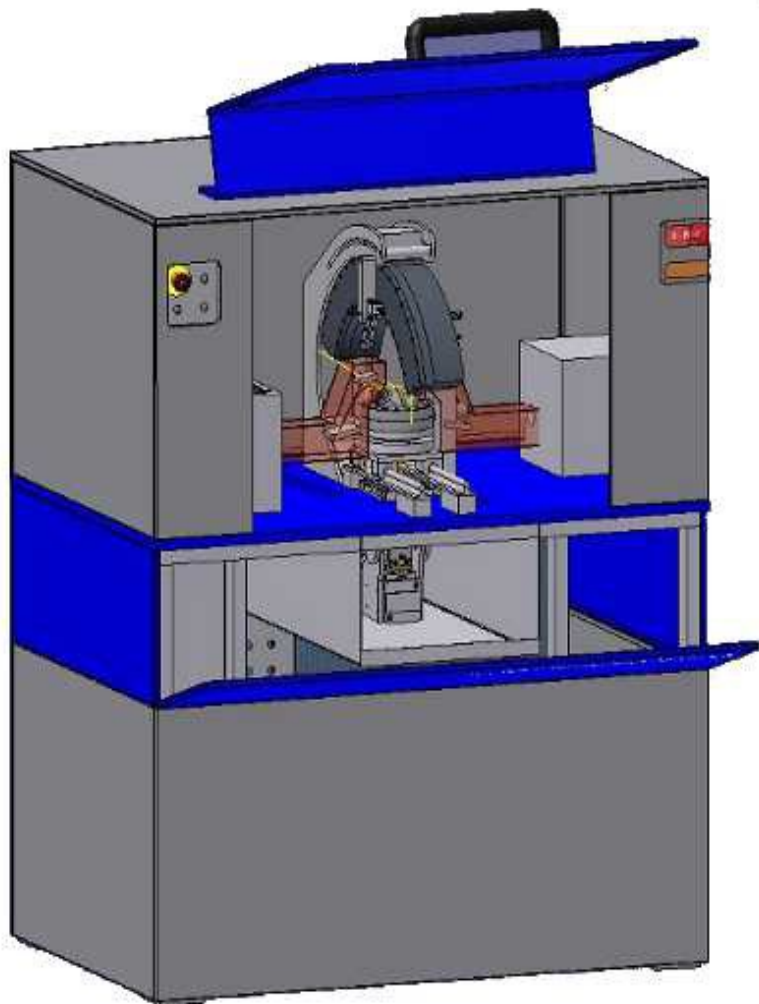
PRECIX

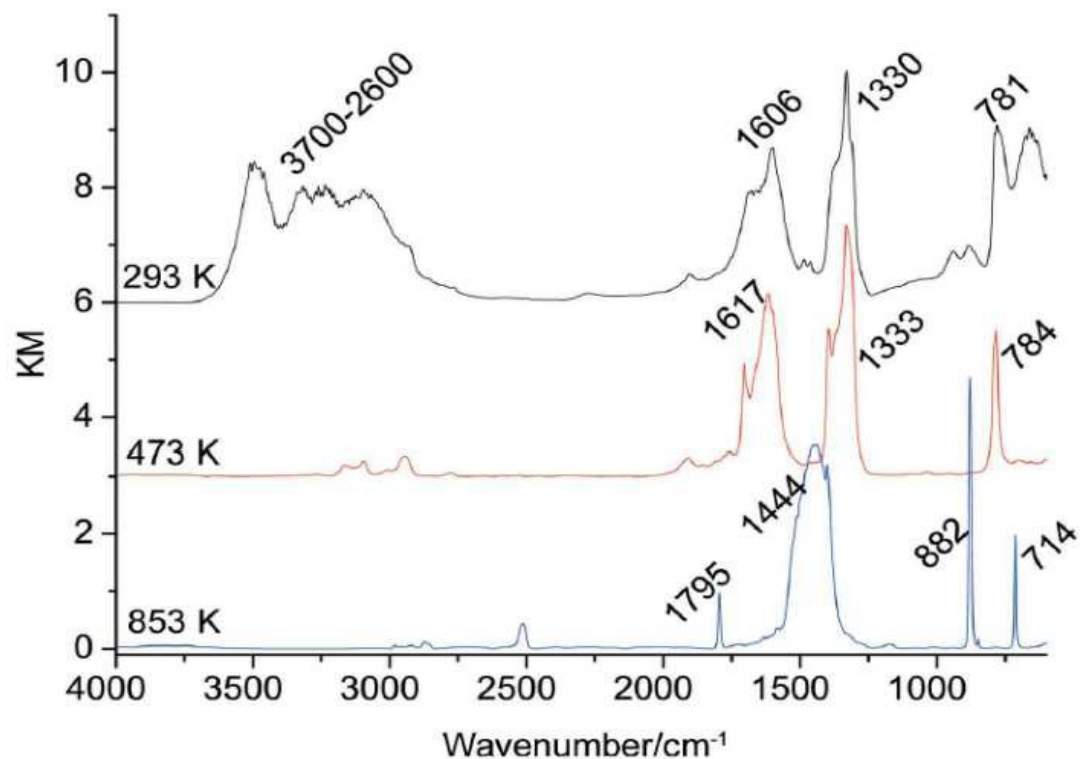
Robotics for XRD residual stress measures



## Phase transitions observation

- Development of a laboratory system, combining XRD and DRIFT, to perform in-situ measurement
- Development of an adapted environmental cell pressure-temperature
- Concept of instrumented system, with an appropriate expert software
- XRD in transmission with Mo radiation
- IR spectrometer in reflection (DRIFT)
- Sample cell with pressure/temperature, and gas mixing.



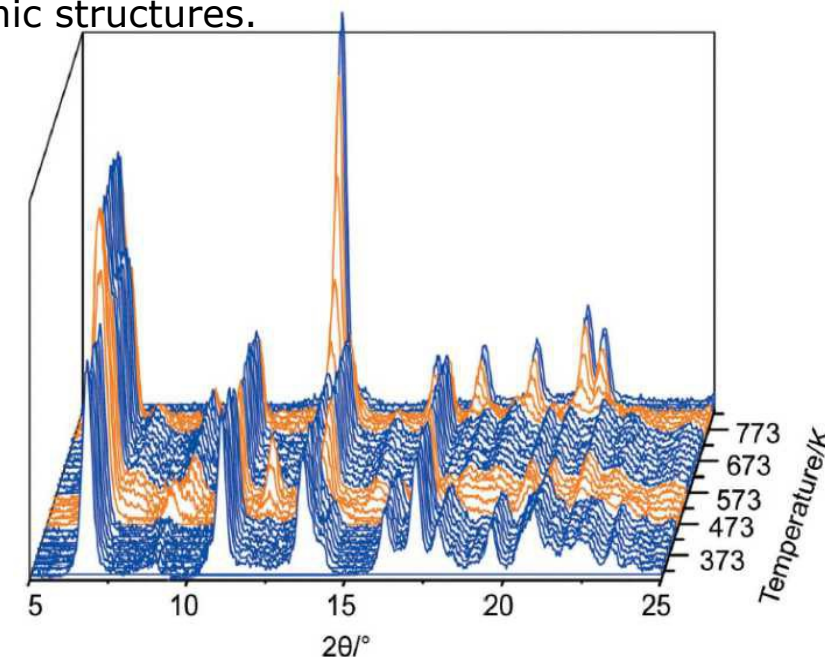


"An X-ray diffractometer coupled with diffuse reflectance infrared Fourier transform spectroscopy and gas chromatography for in situ and in operando characterization: an innovative analytical laboratory instrument", L. Braconnier, I. Clemencon, C. Legens, V. Moizan, F. Diehl, H. Pilliere, P. Echegut, D. De Sousa Meneses and Y. Schuurman, J. Appl. Cryst. (2013). 46, 262–266



DRIFT spectra recorded during thermal decomposition of calcium oxalate (50 mg, 5 Kmin<sup>-1</sup>).

X-ray diffraction patterns recorded during the thermal decomposition of calcium oxalate (50 mg, 5 K min<sup>-1</sup>) Blue traces represent stable crystallographic phases and orange diffraction traces indicate intermediate crystallographic structures.



# Some developments

1997



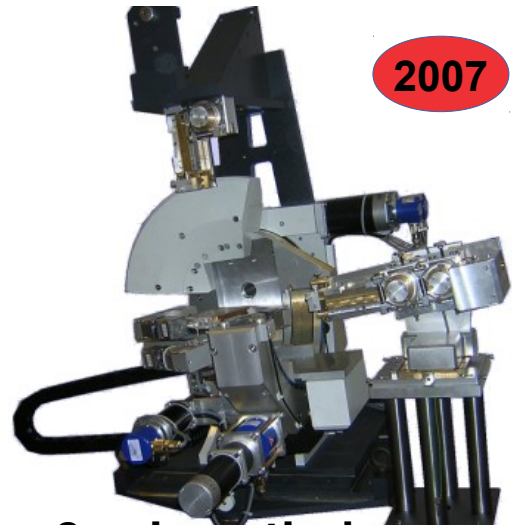
**COSMA, on-line XRD control of cement**

2006



**PRECIX for in-situ stress measurement**

2007



**9-axis vertical goniometer for Epitaxy**

2011



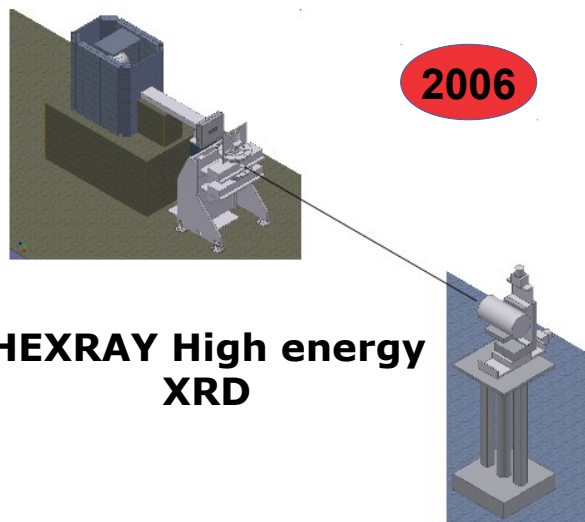
**Stress-Wax combination**

2000



**G3000 4-axis goniometer**

2006



**HEXRAY High energy XRD**

2008



**6-axis horizontal goniometer for Epitaxy**

2010



**XRD-DRIFT combination**

## Interest of combining

- sample is a complicate mixture : XRD+XRF, XRD + Raman
- complementarity to observe phase transition: XRD + IR, XRD + Raman, XRD + DSC
- relationship between mecanical properties and structure : texture + stress
- many other combinations ...

## Advantages

- 1 sample for several measurements, but 1 result
- eliminating non possibilities (XRF prefiltering before search match)
- ...



# Since 2010, wedlock between PSD detector and X-ray minisource

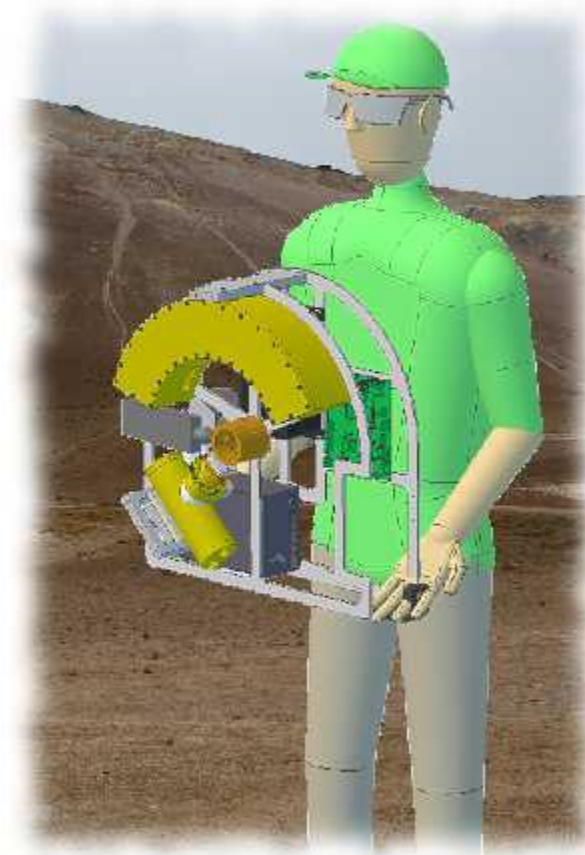
## XRD « escapes » from laboratories

Combining X-ray minisource and CPS detector:

- Low consumption XRD
- Robust instrument
- No external water cooling
- Works on standard power supply

## Inel portable XRD systems:

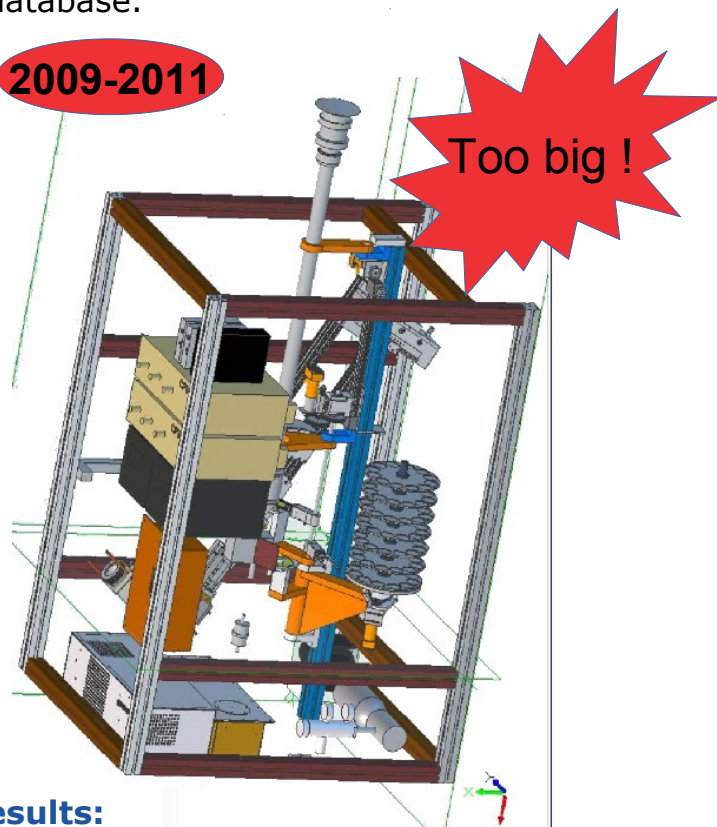
EQUINOX 100	Stand alone benchtop XRD
Enviromonitor	Aerosol quantification expert system
XSOLO	Nomadic Stress System
Equinox Trail	Rackable XRD
SOLXPERT	Portable XRD/XRF system for in field applications



# Granted projects to develop ideas

**Nanoair Project:** (FP7 222333). Design of a prototype, composed by a combination WAXS/SAXS XRD device. Birth of FPSM software (deviation of MAUD), for automatic phases identification and quantification by using the Rietveld method and the COD database.

2009-2011



**Results:**  
Partial feasibility  
New automatic software for data treatment

**Enviromonitor project:** (FP7 SME-2011-3 CP grant agreement N° 286570) for the realization and miniaturization of a mobile system for aerosol sampling and analysis.

2012-2014



**Results:**  
Feasibility in certain conditions  
Performance in miniaturization  
Target market not clearly visible

**Equinox 100:** Bench top XRD



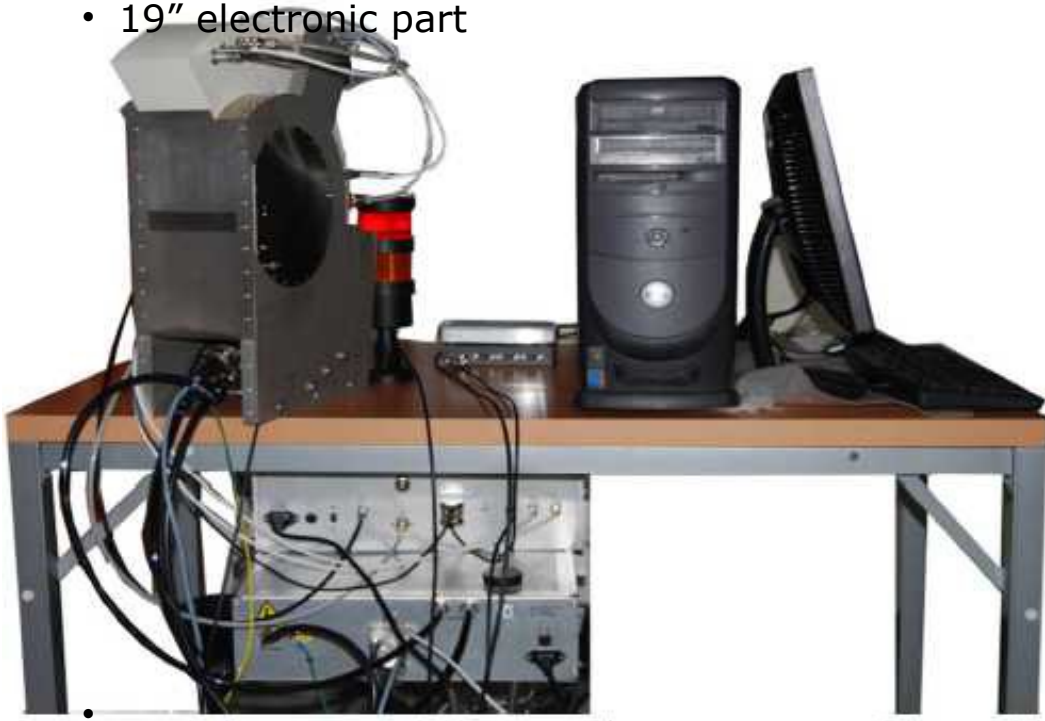
**Secondary results:**  
Optimization of a low power bench top XRD

# Granted projects to develop ideas

## XRD integration in mobile lab

Mobile lab start to be developed, in order to improve the reactivity in the decision.

- Compact instrumental part
- 19" electronic part



## Applications

Environment, geology, police, industry...

## SolXpert, innovation to serve field expertise

Combining XRD-XRF for in-field measurements

Total power : 200 W

## Applications

Environment, geology, police, industry...

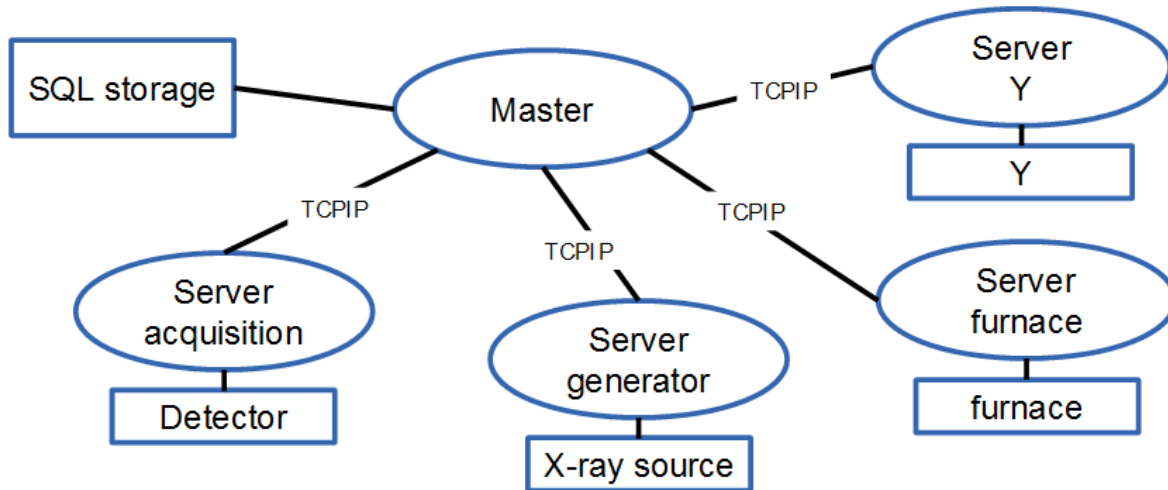


**Goal of software,  
Driving instruments  
And  
Assistance in methodology**

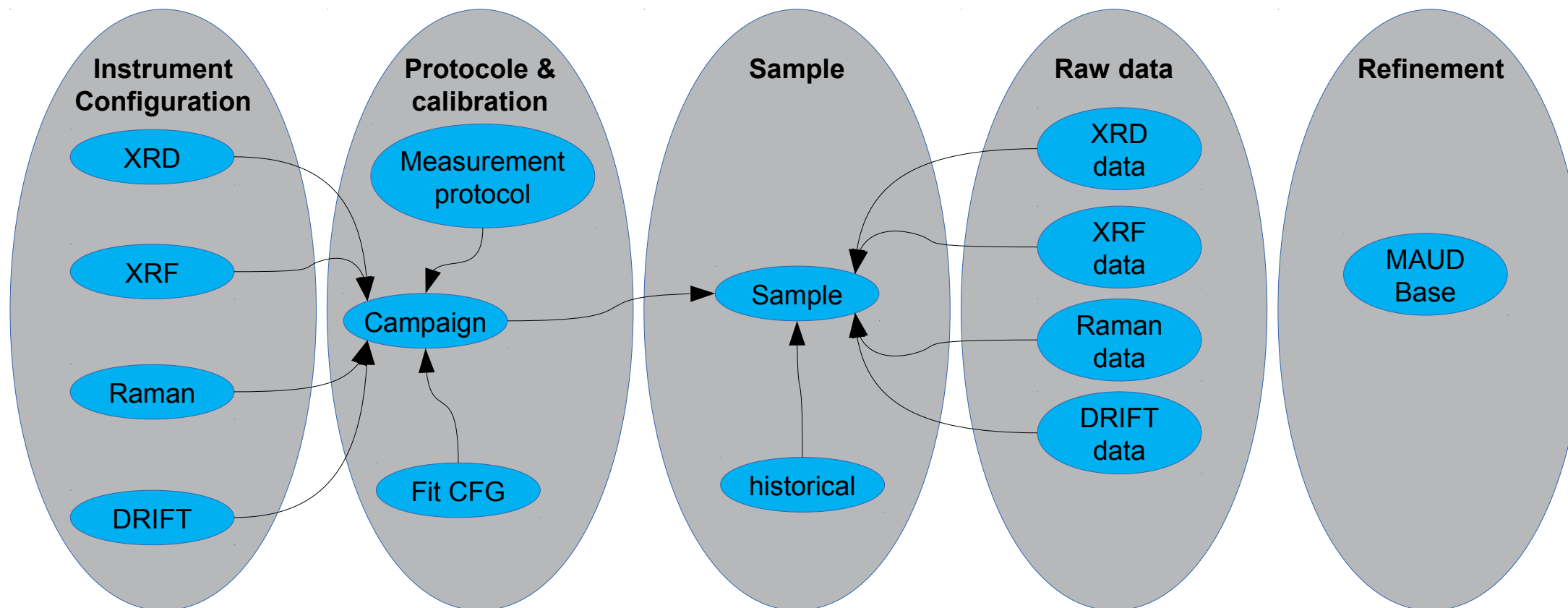
## Development of instrument control software

UNIVERS : from 2013, transition to more universal software :

- data storage (configuration, sample description, raw data and refined data in a unique SQL database)
- sub-programs drive components (servers)
- Master communicates with servers in TCPIP



## Development of instrument control software



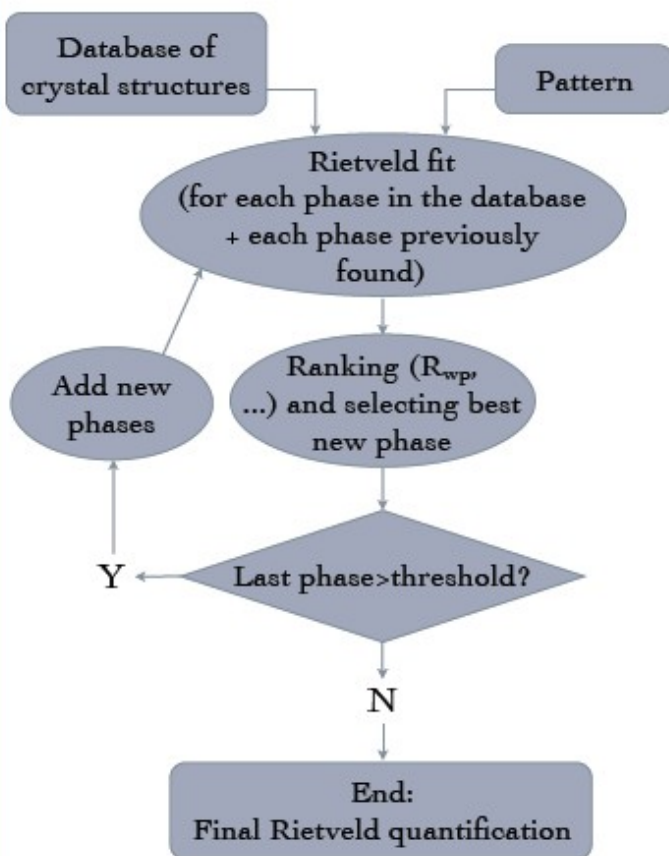
UNIVERS : from 2013, transition to more universal software :

- data storage (configuration, sample description, raw data and refined data in a unique SQL database)
- sub-programs drive components (servers)
- Master communicates with servers in TCPIP

Not yet launched.

## The FPSM (Full Pattern Search-Match method)

Developed inside the Nanoair project for the portable instrument

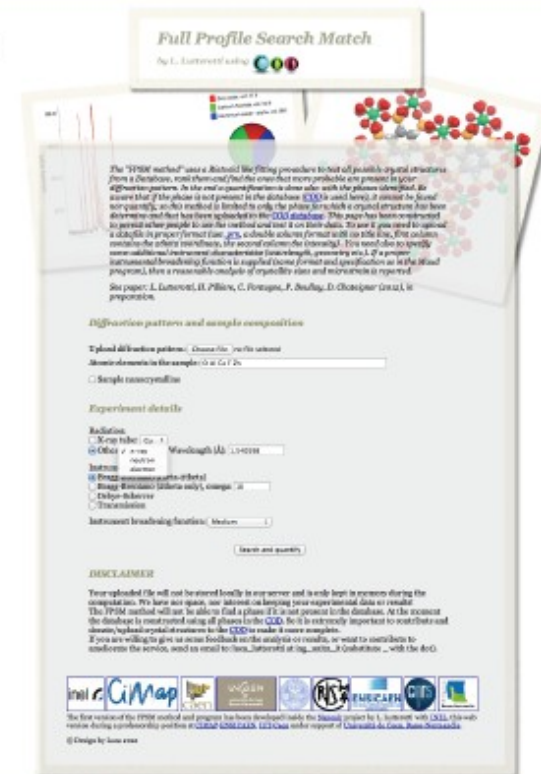


Pro:

- No user intervention, automatic analysis
- No peaks identification required (works with nano materials/particles)
- Full Rietveld quantitative analysis provided
- Works for neutron and electron diffraction

Cons:

- Only phases with known crystal structure are ready to be used (unknown structures require a list of peaks and calibrated intensities, PONKS)
- Available databases are still uncompleted
- If no elemental composition provided → requires > 20 minutes on 12 cores computer
- Good ranking algorithm required for very small phase amount



A demo version has been setup online at:

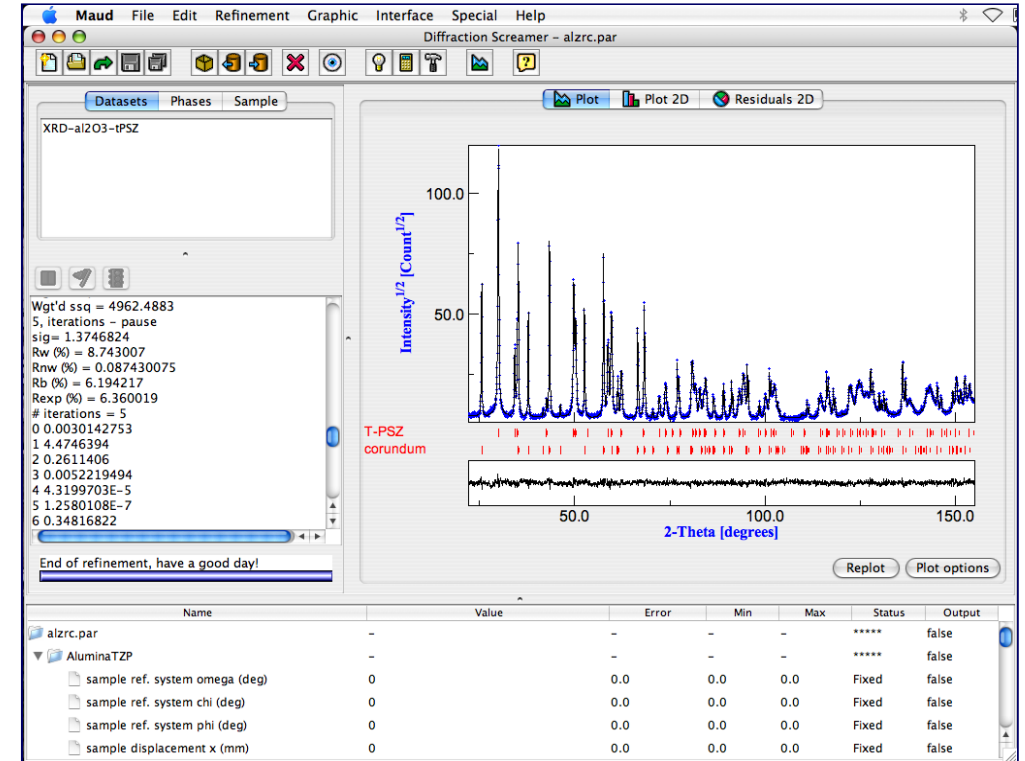
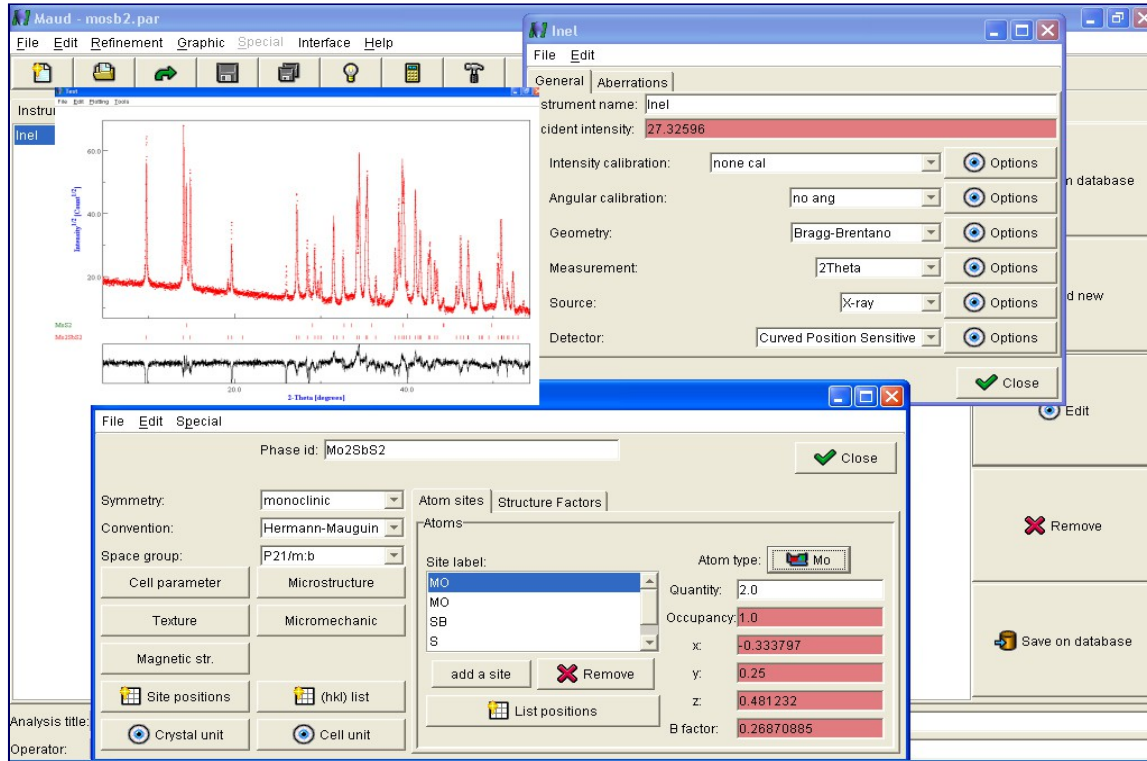
<http://nanoair.ing.unitn.it:8080/sfpm>

search and quantification is limited by the time required (or better server response time) so it should be used restricting the composition as much as possible to speed up computation. A limited number of concurrent connections are supported also. INEL SAS can be inquired for the full version.

See also the demo at the Software Fayre on tuesday afternoon

# Innovative software for Rietveld refinement

## Free software



## Originalities :

- combined refinement with XRD method (powder, texture, stress, grazing ...)
- combined refinement with other techniques (XRF)



- ▶ Light instruments
- ▶ Expert system because of measurement/modeling combination
- ▶ Low power
- ▶ Applications designs
- ▶ Technics combination
- ▶ Unique software for expertize : MAUD



**Thank you for your attention**

*This presentation has been made using only opensource software, so if it didn't work as expected that's normal...*