The Collaboration between Elettra Sincrotrone Trieste

and Zambon Chemicals on polymorphs characterization.

June 6th 2013

XRD1 is a general-purpose, X-ray diffraction beamline characterized by a large energy spectrum, a high flexibility in the experimental set-up and many instrumental solutions in order to be a able to host different kind of experiment:

- Powder diffraction
- Grazing incidence
- *Extreme conditions* experiments *(e.g. high pressure, high temperature)*
- Small molecule structure solution
- Macromolecule (protein) structure solution

(We face very often systems with possible industrial application)

The use of hard X-rays is widespread in industry, in particular in the pharmaceutical one (both in drug discovery/design and in preparation of finite products)

$\Rightarrow$ shared knowledge and languages (accepted methods)

Synchrotrons (more intense X-rays sources and cutting edge instrumentation) can push forward the limits of conventional X-ray sources, opening new opportunities both for industrial process control and for new products.

Polymorphism characterization is based on the capability of X-rays to distinguish among different crystalline forms of the same molecule
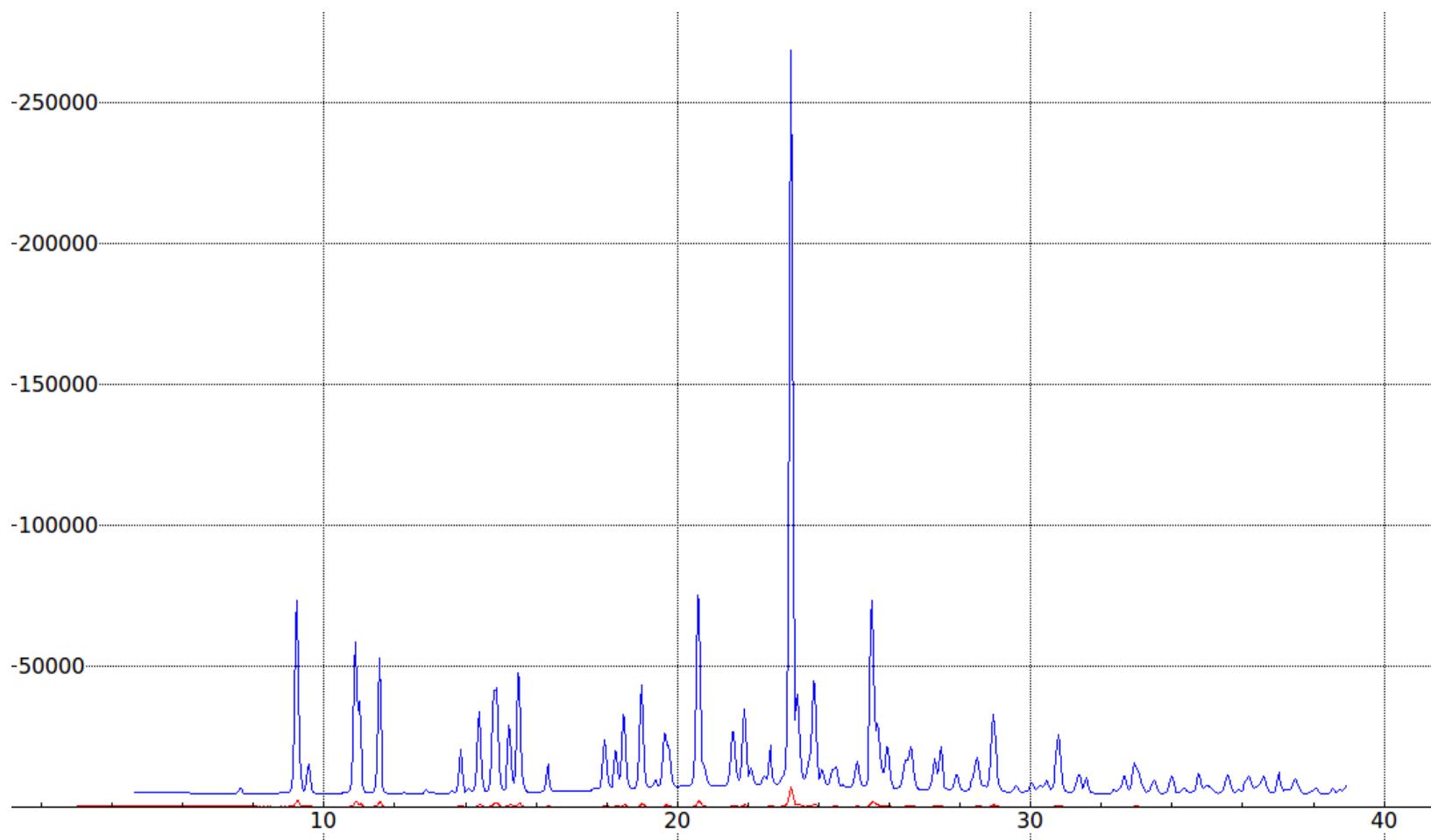
We started from here (2009)...
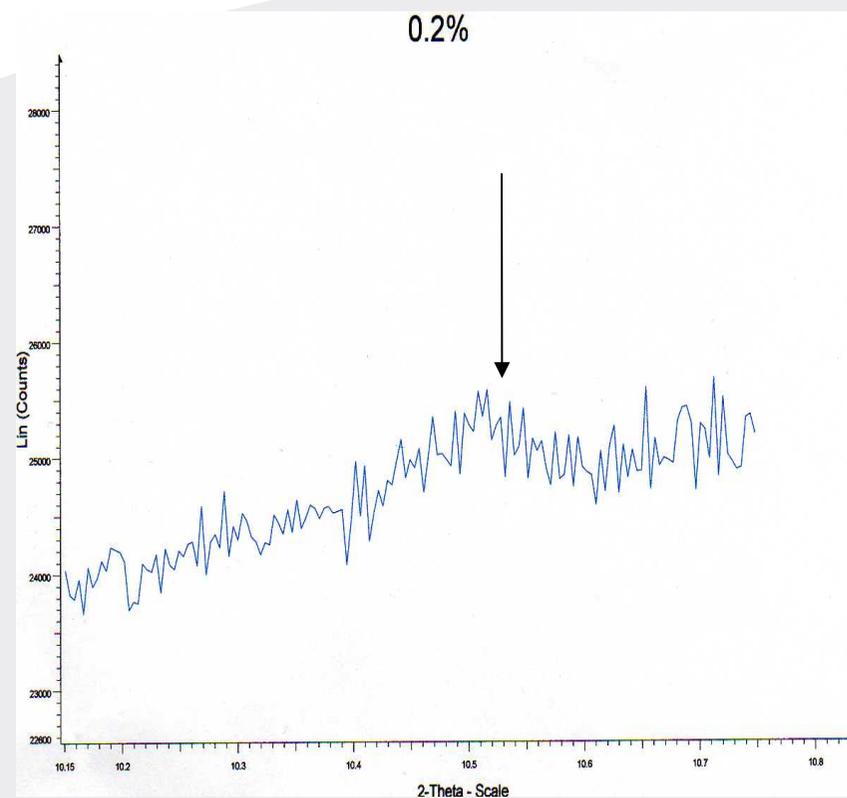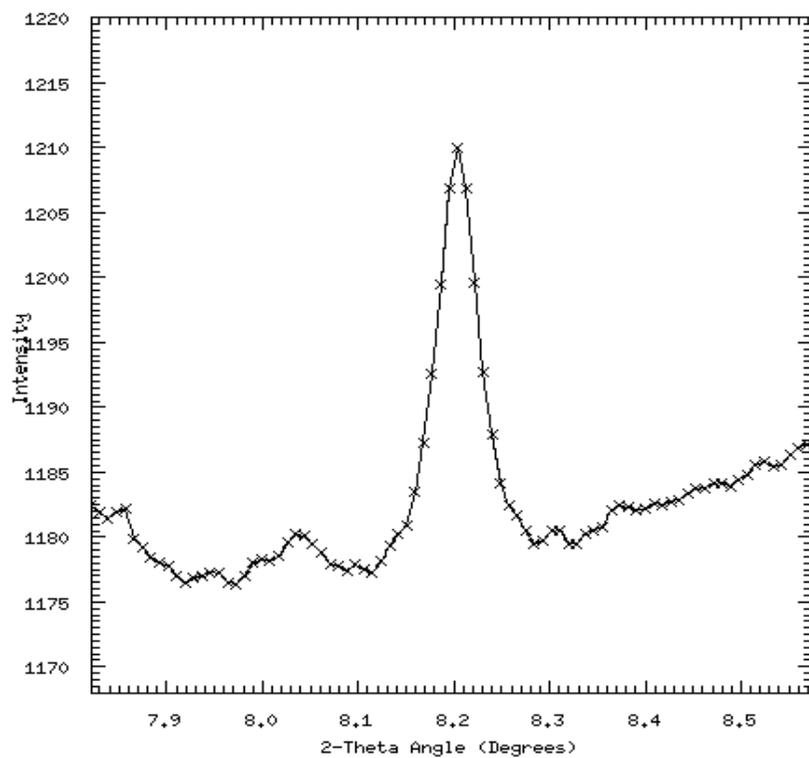
Where we are (long term activities):

- Not only *experiments* but *measures* (long term activities)

⇒ well established procedures/methods (quality and standardization) [tenths of procedures introduced, new methods for data quality indicators, radiation damage evaluation,]

⇒ dedicated processes (e.g. full traceability of samples and data) [2D barcodes for sample automatic identifications]

⇒ optimized technologies (hardware and software) [thousands of software code lines, specific environments for pharmaceuticals samples, safety-related solutions]

⇒ automation (large volumes of measures) [automatic sample manipulation via robotic solution, automatic data collection and analysis]

New opportunities, not considered at the beginning :

- Pushing the known techniques exploiting gained experience

e.g. >> We have been asked to provide methods to improve the Limit of detection, up to 50 ppm or lower

- New technologies to overcome specific problems

e.g. >> We develop new methods/algorithms (patent) for data quality estimation/quantification,radiation damage evaluation, noise reduction for improved data quality, process control

- new opportunities for business

e.g. >> Finite product test: measures of the pills content in the blisters (final quality control, anti-counterfeiting, competitors quality)

Thanks for your attention