XALOC: A Flexible Macromolecular Crystallography Beamline

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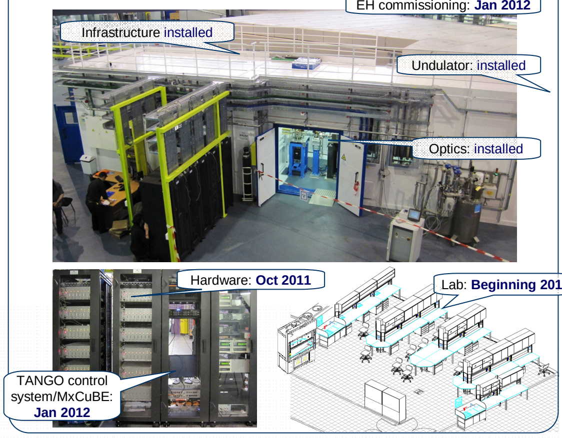
Scientific case

X-ray crystallography has emerged as a very effective technique to perform 3D structural studies on biomolecules at the atomic level.

In response to this, one of the phase-I beamlines (**XALOC – BL13**) of the third generation **3-GeV synchrotron Alba** will be devoted to Macromolecular Crystallography.

Overall status



XALOC is a versatile beamline

…for many techniques

- All wavelength-dependent techniques can be performed (MAD, SAD, etc) due to the **full-wavelength tunability** and the high resolution ($\Delta\lambda/\lambda$~2 10^{-4}) of the beam,
- All common **K and L_3 absorption edges** are reached: 2.4–0.6 Å or 5–21 keV. Covered elements are: V➔Mo (K); La➔ U (L_3),
- An in-vacuum undulator provides a **high-flux beam** (>2x10^{12} ph/s) over the whole energy range

Specifications of the in-vacuum undulator (IVU21)

Period (number of periods)	21.6 mm (92)
K (at minimum gap, 5.5 mm)	1.60
Photon source size (h×v, FWHM)	309 × 18 μm^2
Photon source div. (h×v, FWHM)	112 × 30 μrad^2

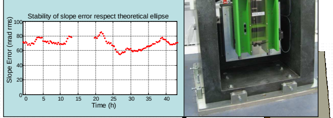
Undulator IVU21

…for many crystal types

- **Small crystals** can be studied by **focusing** the beam down to **~50×10 μm^2** (h×v) with a beam divergence of **0.5 ×0.1 mrad^2**,
- **Any medium-sized crystals** can be dealt with by **defocusing** the beam up to **~300×100 μm^2** (h×v),
- **Larger crystals** can be completely exposed to the x-ray beam by **unfocusing** the beam to **~500×500 μm^2** (h×v). This beam is also highly vertically collimated (**0.03 mrad**) and hence it can be used for crystals with **very large unit cells** like protein-protein complexes, viruses, etc.

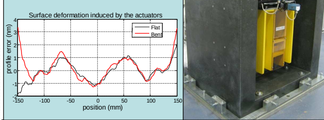
Horizontal Focusing Mirror

- 600 mm optical surface
- Bare Si, Rh, and Ir coated
- 83 nrad slope error (bent)
- 3 Å roughness



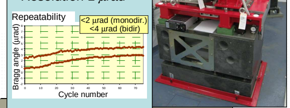
Vertical Focusing Mirror

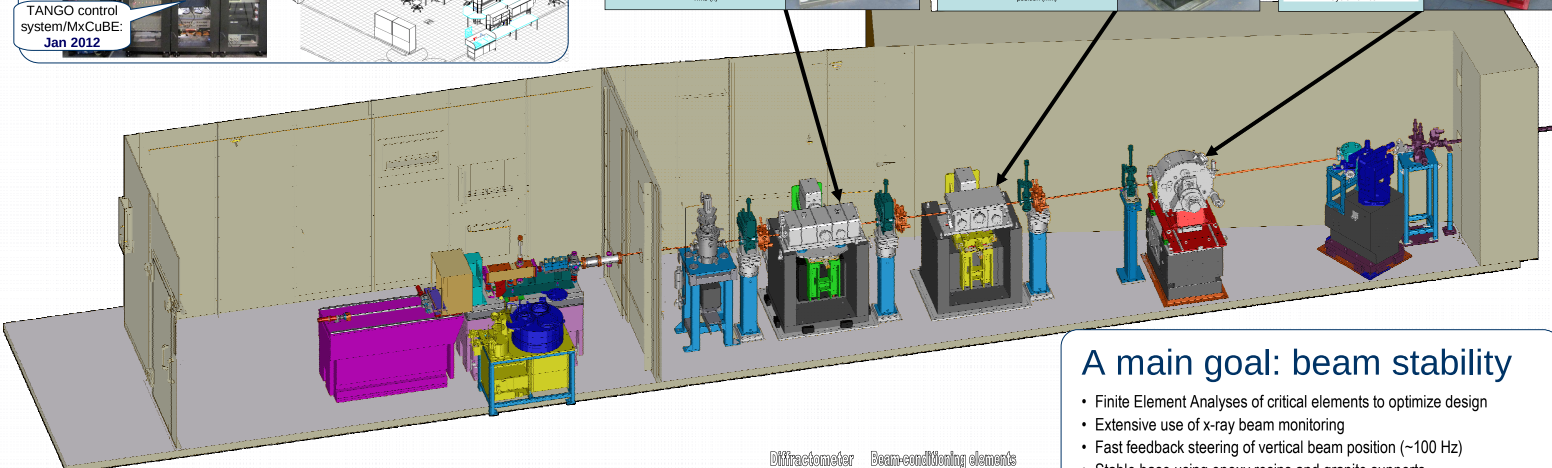
- 300 mm optical surface
- Bare Si, Rh, and Ir coated
- 70 nrad slope error (bent)
- 3 Å roughness



Monochromator

- Si(111) channel-cut
- Liquid N_2 cooled
- Fast V beam steering
- Stability <0.05 eV/h
- Resolution 1 μrad





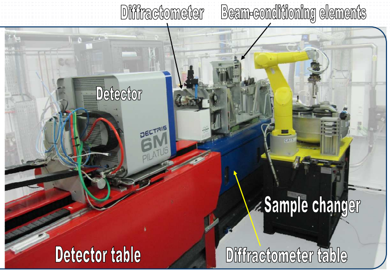
A main goal: beam stability

- Finite Element Analyses of critical elements to optimize design
- Extensive use of x-ray beam monitoring
- Fast feedback steering of vertical beam position (~100 Hz)
- Stable base using epoxy resins and granite supports
- Strain gauges in mirror benders to stabilize focusing
- Seismographs close to optical surfaces to deal with vibrations

End Station: the concept

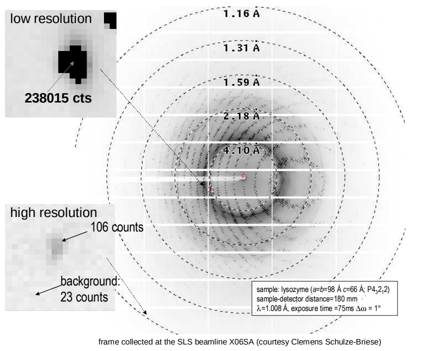
The End station consists of two in-house developed translation/rotation tables that support the diffractometer and the detector sitting on a granite base. The tables are adjustable to 1 µm resolution and repeatability.

An automatic sample changer stands on a nearby table for automatic sample mounting and allows easy access to manual mounting.



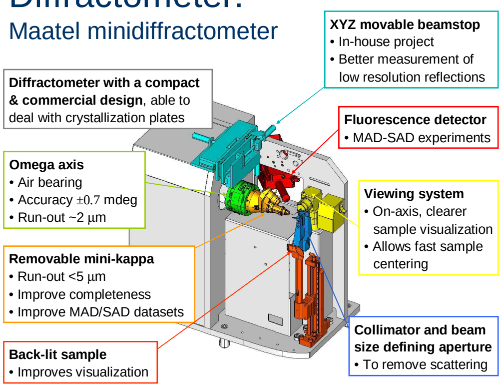
Detector: Dectris Pilatus 6M

- **High dynamic range** (1 million): collection of low and high resolution data on the same frame
- **Extremely low background noise**
- **Fast read-out**: shutterless collection, minimizing systematic errors
- **Thin ω-slicing** which often results in better data in high-resolution data and large unit cell crystals
- **Fast frame collection** (80ms/image): a 360º 1.1 Å resolution dataset can be collected in 33 seconds



frame collected at the SLS beamline X06SA (courtesy Clemens Schulze-Briese)

Diffractometer: Maatel minidiffractometer



Sample changer: Irelec CATS for SPINE pins & cristallization plates