CoSAXS *

External collaborations	RÅC grant, SOLEIL-MAX IV collaboration
Original budget and funders	Investment budget: 97.0 MSEK, SRC
Official start	February 2014
Expected date of completion:	2018 open for external user

In soft matter and many biological systems one typically deals with structures occurring on the so called colloidal length scale ranging from nanometre up to micrometres. Small-angle X-ray scattering (SAXS) is ideally suited to investigate hierarchical, heterogeneous and complex structures. X-ray Photon Correlation Spectroscopy (XPCS) deals with the underlying cause of the structural evolution over time, i.e. dynamics. Hence, an instrument, which provides SAXS and XPCS in a complementary form, has a large and broad user community from essentially the whole range of scientific disciplines.

The CoSAXS beamline promotes new studies and developments in hierarchically self-assembled soft matter and nanostructured materials with studies over a unique range of simultaneous length and time scales. Experiments performed at the CoSAXS beamline will be able to exploit the unprecedented properties of the MAX IV source: the high brilliance, and the high degree of coherence of the beam.

Because of the very broad user community, this first SAXS beamline at MAX IV is a multipurpose instrument. In order to secure the state-of-the art performance for a wide range of applications, the instrument is carefully designed and requires highly qualified dedicated staff to provide the necessary range of competence.

Technical description

Design goals:

- Energy range: 4 to 20 keV; with the main working energy at 7.1 and 12.4 keV. Energy resolution: $2x10^{-4}$
- Photon flux 10^{13}-10^{12} ph/s with variable and independent horizontal and vertical focusing.
- Coherent photon flux of 10^{11}-10^{12} ph/s with adjustable aperture collimation.
- Scattering vector q-range: $6x10^{-4} \leq q \leq 6$ $Å^{-1}$ at 12.4 keV (d-values: 1 000 to 0.1 nm) with simultaneous SAXS/WAXS detection. q-resolution: 10^{-4} $Å^{-1}$ or better for specific configurations (typical q < 1x 10^{-3} $Å^{-1}$)
- Typical beam sizes at the sample of ~100x100 µm^2. Possibilities of spot size of ~10x10 µm^2
- Multiple techniques: solution and solid state SAXS, BioSAXS, time resolved SAXS (TR-SAXS), SAXS/WAXS, Coherent hard X-ray scattering, Anomalous SAXS (ASAXS). Multiple and complex sample environments.

Technical implementation:

X-ray source (IVU)	In-vacuum undulator (IVU), 2 m magnetic length, 19.3 mm period, 101 periods, 4.2 mm minimal magnetic gap.
Energy (wavelength) range	4 - 20 keV (0.6 – 3.1 Å) using 1st - 11th harmonics of the IVU
Monochromator (hDCM)	At 25 m, Si (111), double crystal monochromator, horizontally deflecting, inclined crystals, LN_2 side-cooling.
Energy bandwidth (ΔE/E)	~2 x 10^{-4} (Si 111 band)
Focusing optics	Dual Kirkpatrick-Baez (KB) mirror pair ($VFM_{1,2}$ and $HFM_{1,2}$) in four bounce geometry.
Vertical mirrors pair (VFMs)	At ~27 and 28 m, flat surface, 400 mm length, 0.1 µrad RMS slope error. Both are bendable flat mirrors. VFMs can be retracted from the beam.
Horizontal mirrors pair (HFMs)	At ~29 and 30 m, 400 mm length, 0.1 µrad RMS slope error. Both are bendable flat mirrors.
Harmonic rejection	HFMs and VFMs with Si (uncoated) and Rh stripes.
End station and detectors	18 m flight tube. In vacuum compatible 2D pixel hybrid detectors for simultaneous SAXS/WAXS

Present status

ID and main optical components: procured and in production. Optical and experimental hutches: construction finished. Infrastructure: defined (3D drawings and time plan) and installation initiated. SAXS/WAXS chamber (flight tube): design phase, to be procured in autumn 2016. End station: experimental table and basic sample

* https://www.maxiv.lu.se/accelerators-beamlines/beamlines/cosaxs/

environment under design and prototyping. IT: basic operation design. Prototypes for data reduction software. Staff: one project manager, one beamline scientist, one temporary position (ending in Dec 2018).

Expected status end 2018

- User operation with a limited amount of techniques and sample environment available. Main available techniques: solution and solid state basic SAXS, BioSAXS, 2D mapping SAXS. IT: basic on fly- data analysis; robust data reduction software; basic data modelling software.
- Advanced status for the implementation of SAXS/WAXS and time-resolved experiments.

Major partners and additional funding

Funding: (i) Röntgen Ångström 2015 (Main collaborator: G. Katona (GU). 2014 kSEK *funded to CoSAXS*; Co-PI: T. Plivelic. (ii) SOLEIL-MAXIV collaboration. *Main collaborator: J. Perez (SOLEIL).* : 201.1 kSEK *funded to CoSAXS-SWING beamlines* PI-resp.: T. Plivelic.
Partnerships: A large group of local or international collaborations has been settled for scientific or instrument related projects within the CoSAXS beamline. Principal beamline partnerships (in kind): N. Tirrell (Diamond); M. Krumrey (Bessy-II); E. DiMasi (NSLS-II), J. Perez (SOLEIL), M. Sprung and C. Blanchet (Petra III).

Changes made since the start

The optical design of the beamline has been modified in order to make better use of the source properties and to increase the flexibility (towards: wave front preservation, independent vertical and horizontal focusing in the full path of the beamline and micro-beam possibilities).

The use of coherent hard X-ray scattering experiments will be implemented through X-ray photon correlation spectroscopy (XPCS) with the collaboration from experts in the field, but only after the SAXS technique has been secured, as was decided by the advisory committee (STAP) in October 2014.

The developments of the CoSAXS beamline towards life science experiments have been strengthened with the addition of Time Resolved SAXS experiments (TR-SAXS; from ms to µs time resolution) in biological samples in solution, from earlier commissioning (2017-2018, see also RÅC grant).

The beamline time plan is roughly as initially proposed. However, we have extended the period of expert commissioning users up to Q1-Q2 2018. External users at CoSAXS are expected during 2018.

Comparison to beamlines world wide

ID02 at ESRF (France): http://www.esrf.eu/UsersAndScience/Experiments/CBS/ID02
P12 at Petra III (Germany): http://photon-science.desy.de/facilities/petra_iii/beamlines/p12_biosaxs/index_eng.html
cSAXS at SLS (Switzerland): https://www.psi.ch/sls/csaxs/

Future development

The initial period after 2018 should be used to strengthen the multipurpose character of the beamline on the SAXS/WAXS techniques, adding expertise and suitable complex sample environments on soft matter and life science related subjects (for example combined spectroscopy and SAXS (SURF), tensile and shear test machines, microfluidics). Time Resolved SAXS should also be developed at the beamline, through external user's demands and in-house expertise. We will also invest to better characterise the potential of the beamline on micro -beam possibilities (down to 10 x 10 μm^2).

In the middle to long run, XPCS primarily, and ASAXS experiments, can also be implemented, and spread around the user community. XPCS brings the opportunity to study the underlying dynamics in nanostructured complex fluids whereas ASAXS determines position and organisation of specific elements in macromolecules in solution or industrial catalyst.