Expression Of Interest (EOI) for XPCS experiments at MAXIV

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MAXIV is currently the most brilliant synchrotron source in the world thanks to its innovative Multi-Bend Achromat (MBA) design. One of the hallmarks of MBA sources is the two order of magnitude increase in coherent X-ray flux, extending also into the higher photon energies beyond 10 keV, as compared to lattice designs of conventional storage rings. Among the different techniques available at synchrotron sources, **X-ray photon correlation spectroscopy (XPCS) benefits particularly from the related boost in brilliance B_r,** allowing an improvement of the signal-to-noise ratio of the measurements by a factor of 100, as well as accessing correlation time-scales much faster than previously possible. In fact, the fastest accessible time scales in XPCS experiments scale as $\tau \sim 1/\,{B_r}^2$; hence, MAXIV promises to explore temporal regimes which are up to four orders of magnitude faster. Moreover, the increased spatial coherence length allows decreasing the photon density on the sample. This makes experiments on radiation-sensitive samples feasible, which **opens up the rich field of biophysics for XPCS.**

1. Motivation

During a **dedicated session on coherent scattering with around 100 participants,** followed by a round table discussion at the **MAX IV Users Meeting 2019**, the international user community discussed the scientific perspectives of using the superior coherence properties of MAX IV for performing XPCS experiments. Based on those discussions and the input from the users we decided to formulate this "Expression of Interest" (EOI) outlining the unique science case and documenting the interest of the international community. The letter is intended for the management of MAX IV, indicating in addition a set of desired parameters for a dedicated XPCS beam line. Finally, we suggest commissioning steps for such experiments at MAX IV, invoking also the expertise of international XPCS expert users and facility members.

2. Science Cases

In the science session we have identified and discussed several science cases, both of fundamental and applied interest, that utilize XPCS across the scientific fields. Here we mention some of the examples that would considerably benefit from the **superior coherent properties of MAX IV** for capturing dynamics with XPCS. These include:

- Protein dynamics in crowded environments and biomolecular condensates
- Dynamics of water and aqueous solutions
- Dynamics in nanostructured liquids, such as ionic liquids, highly concentrated electrolytes, and hydrogen bonded systems
- Glassy dynamics and polyamorphism at high pressures
- Phase transitions and critical non-equilibrium dynamics
- Fluctuations of magnetic, ferroelectric and other order parameters in condensed matter
- Fluctuations in high-T_c semiconductors
- Atomic motion in glass formers, both in bulk and surfaces
- Aging mechanism in organic electronics
- Surface dynamics for epitaxial film growth and corrosion layer development
- Nanocellulose dynamics, confined polymers
- Pattern formation, material deformation and oscillatory reactions
- Sheered suspensions *in situ*, nanofluidics
- Anisotropic diffusion under external fields and driven self-assembly.

3. Experimental Parameters

In addition, we discussed experimental parameters that would be required for performing XPCS experiments as well as the appropriate steps for commissioning of an XPCS-dedicated beamline (*e.g.* CoSAXS). One of the most important points discussed was that it is essential to make a recruitment with previous XPCS experience, who would push this technique forward from the beamline side, in addition to the external assistance from the user community and international experts. The **experimental parameters discussed and regarded as pivotal for performing XPCS experiments** are as follows:

a. Highly stable and coherence-preserving optical elements
b. Requirements of photon transport and X-ray optics such as flat mirrors, apertures, flexible focusing options via compound refractive lenses (CRL) for adapting photon densities and speckle contrast, guard slits, flexible sample-detector distances for matching speckle and pixel sizes
c. Fast (microsecond and below) pixelated X-ray detectors
d. Data analysis pipeline for coping with the large amount of data produced in XPCS experiments, user-friendly software, and efficient data-compression schemes.
e. Beam monochromaticity capabilities such as Si(111), Si(331) or higher.
f. Sample environments with temperature control (80K – 450K), laser and magnetic field capabilities, mechanical stress, pressure and microfluidic cells.

4. Commissioning plan for XPCS

Noting that CoSAXS is foreseen for XPCS experiments, we envision a commissioning plan for XPCS capabilities which includes the following steps:

1. Speckle tests from static reference samples such as aerogels etc.
2. Simple colloidal dynamics for testing beamline components/stability/software
3. Large Q-tests for stability and contrast determination
4. XPCS performance comparison with P10 at DESY, 8 ID at APS, 11-ID at NSLS-II and ID10 at ESRF
5. Theoretical SNR expectations for an XPCS end station at MAX IV.
6. Invoking a small international technical advisory board from international facility experts with XPCS beam line experience to revise commissioning and propose future actions.

The XPCS user community is willing to support this effort with **user-assisted commissioning** in collaboration and with **support from international XPCS experts**.