

XPCS workshop report, 6-7th June 2018

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This was a lunch to lunch workshop to identify some of the challenges facing the advancement of X-ray Photon Correlation Spectroscopy (XPCS). This technique allows access to the dynamics of molecules on the timescale of relevance to the study of the diffusion, relaxation etc. in a sample. As such it has been applied in condensed matter systems, for example in glasses, but is under-exploited in biological samples where it could bridge the gap between neutron spectroscopy and light scattering. The technique examines the temporal variation in the coherent speckle pattern from a sample where there are spatial inhomogeneities present. As such, it will benefit greatly from the new synchrotron X-ray sources that will provide high coherent flux. These facilities are either nearing operation (CoSAXS at MAX IV) or about to be upgraded to deliver higher coherent flux (ESRF and APS), thus there is a timeliness to exploring what needs to be done to develop the potential of XPCS to move from idealized samples to address relevant scientific questions. It is apparent that difficulties to be addressed include: detector speed, signal to noise and beam damage. For this reason, a small group of selected experts who cover all the relevant areas were invited to Lund for an informal discussion of the practicalities of such measurements and the developments which are needed. The following attended the meeting.

Larry Lurio, Northern Illinois Uni
Christian Gutt, Uni of Siegen
Yuri Chushkin, ESRF XPCS Beamline
Michael Sprung, Petra III XPCS
Felix Lehmkühler, Petra III
Anders Madsen, European XFEL XPCS Beamline
David Pennicard, Petra III Detector Group
Nicolas Pilet, Dectris Detectors
Antara Pal, Lund University
Peter Schurtenberger Lund University
Felix Roosen-Runge, Lund University
Anna Stradner, Lund University
Ann Terry MAX IV
Tomás Plivelic, MAX IV
Kim Nygård, MAX IV

Summary of Discussions

The discussions were very frank and open but also proved highly informative as to the current state of the art for XPCS. The potential of the technique was clearly presented in a few examples but the ability to expand this to wider scientific problems requires the addressing of certain experimental issues as well as the identification of the key scientific questions which XPCS will show the most gains over neutron techniques. It is clear that some difficulties still need to be overcome, for example, detector speed. The two representatives for detector development were already aware of the need for increased speed etc and there are two possible developments, both in Europe, which have potential for very big gains. However, generally there will be more future improvements but not in the short term. Issues

like radiation damage can be circumvented with appropriate sample environment and strategies for data collection. However, data interpretation is still a bottle-neck in most experiments requiring expert support and thus is not open to the general user. The underlying code used by all the facilities is basically the same, however, there is very great room for improvement.

The overheads for all the presentations will be made available.

What LINXS can do?

In the short term, LINXS should host further discussions and workshops between the interested parties. It is clear that only such a concerted effort may bring the necessary advances and all the parties wanted such a forum to raise the profile of XPCS. The new/upgraded sources, with their higher coherent flux, have great potential to bring significant gains to the technique, however effort is required now. It was felt that some annual Europe-wide meeting might prove the most useful. Only by unifying the need for, for example, increased detector speed, will enough pressure be brought to drive the needed development.

LINXS should also investigate how the software for analysis can best be updated or supported, perhaps by hosting the right people within LINXS for such a task. Additional funds will be needed for any recruitment to accomplish this. LINXS would be able to coordinate such an application.