PAUL SCHERRER INSTITUT

PHOTON SCIENCE - SEMINAR

A split-beam Probe-Pump-Probe scheme for femtosecond time resolved protein X-ray crystallography

Jasper J. van Thor

Imperial College London, UK

DATE: Friday, 31 October 2014
Coffee: 11:00 h
SEMINAR: 11:15 h
PLACE: WBGB/019

Abstract:
In order to exploit the femtosecond pulse duration of XFELs operating in the hard X-ray regime for ultrafast time-resolved protein crystallography experiments, critical parameters that determine the crystallographic signal-to-noise ($I/\sigma I$) must be addressed, as well as femtosecond photochemical dynamics which may limit transient population level (Lincoln et al., 2012). For single-crystal studies under low absorbed dose conditions, it has been shown that the intrinsic pulse intensity stability as well as mode structure and jitter of this structure, significantly affect the signal-to-noise and crystallographic accuracy (van Thor et al., 2014). Geometrical parameters are explored for a three-beam scheme: X-ray probe, optical pump, X-ray probe (or 'probe-pump-probe') which will allow experimental determination of the photo-induced structure factor amplitude differences, ΔF, in a ratiometric manner, thereby removing the noise characteristics of the source from the measurement. In addition to a non-collinear split-beam geometry which separates un-pumped and pumped diffraction patterns on an area detector, applying an additional convergence angle to both beams leads to integration over mosaic blocks in the case of well ordered protein crystals. Ray-tracing X-ray diffraction simulations are performed for an example using Photoactive Yellow Protein crystals in order to explore the geometrical design parameters which would be needed. The experimental parameters for an X-ray split and delay instrument that implements both an offset angle and convergent beams are discussed, for implementation of a probe-pump-probe scheme at the European XFEL. A possible extension of single crystal studies to serial femtosecond crystallography will be discussed, particularly in view of the expected X-ray damage due to the first interaction.

Contact: Chris Milne (5477)