

MS44-1-3 Ultrafast X-ray diffraction and scattering on the Femtosecond X-ray Experiment (FXE) instrument at the European XFEL: present status and future perspectives

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Abstract

Time-resolved X-ray methods are widely used for monitoring time-resolved electronic and structural dynamics over the course of photochemical reactions. Since fundamental processes in physics, chemistry and biology occur in ultrashort time range (from 10^{-12} to 10^{-15} s), X-ray free electrons lasers (XFELs) development received much more attention in the last ten years. Several experiments have successfully demonstrated that this new generation of light sources provides unprecedented insight into structural and electronic dynamics occurring during photo-induced reactions in various condensed-matter systems [1-2]. The EuXFEL allows to investigate these types of mechanisms thanks to the extremely brilliant ($>10^{12}$ photons pulse⁻¹), ultra-short pulses (<100 fs), transversely coherent X-ray radiation, high repetition rate of up to 4.5 MHz, and extreme focusing (<10 μ m).

In this contribution, we present an overview of the present status and future perspectives of time-resolved diffraction and scattering techniques at the FXE beamline in EuXFEL. The instrument uses femtosecond optical laser pulses to pump the samples while the ultrafast X-ray FEL pulses probe their dynamical evolution in the so-called pump-probe method. The FXE instrument enables a femtosecond temporal resolution down to about 115 fs FWHM [4]. One unique scientific capability of FXE is to study ultrafast dynamics with various X-ray methods simultaneously in the photon energy range from 5 to 20 keV [3-4]. X-ray diffraction and scattering experiments on liquid and solid systems have been achieved at FXE [3]. For instance, ultrafast photochemistry studies in solution phase are performed by combining the wavelength-dispersive 16-crystal von Hamos X-ray emission spectrometer (XES) and X-ray solution scattering (XSS) recorded the Large Pixel Detector (LPD) [5-6]. Starting with non-resonant simultaneous Ka and Kb XES on Fe complexes [7-9] the capability was extended to a variety of other metal complexes including Co-, Ni- and Cr-based systems. The FXE beamline have also achieved successful solid-state experiments, including XES on thin films, single-crystal XRD with the Jungfrau detector motion, and polycrystalline scattering with the LPD.

The next step at the FXE beamline is to enable further solid-state experiments. In this perspective, the XTRAS project (ultrafast X-ray crystallography with diverse sAMple delivery) will be developed to provide femtosecond atomic "movies" of molecular crystals by means of single crystal XRD experiments and to reconstruct ultrafast intermediate state structures. The objective is to upgrade the existing vacuum chamber, and thereby provide rotation XRD, simultaneous XRD and XES, and cryogenic conditions for experiments requiring diverse sample delivery methods.

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