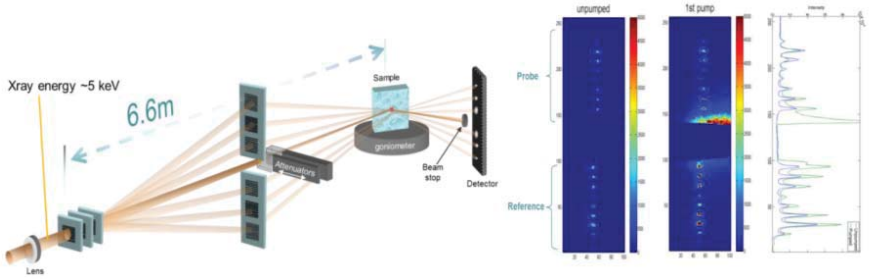

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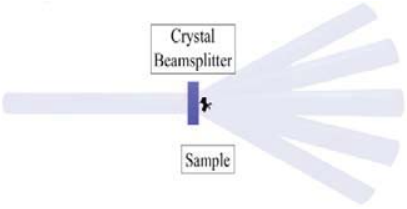

Towards XFEL

Tuesday, April 19th, 2016

10:00 to 12:15, WBGB/019

10:00 Fixed target approach to time-resolved measurements on protein crystals at Free Electron Lasers.
Nadia Opara, Thomas Braun, Henning Stahlberg, Mikako Makita, Christian David, Celestino Padeste

10:30 Single-shot & time resolved, x-ray-pump & x-ray probe method for ultrafast dynamics
Mikako Makita, I. Vartiainen, I. Mohacsi, A. Diaz, P. Juranic, A. Meents, C. Milne, A. Mozzanica, N. Opara, C. Padeste, V. Panneels, M. Sikorski, S. Song, P. Willmott, L. Vera and C. David

11:00 Coffee

11:15 AGIPD: A High Frame Rate Detector for the European XFEL
Davide Mezza, A. Allahgholi, A. Delfs, R. Dinapoli, P. Goettlicher, H. Graafsma, D. Greiffenberg, M. Gronewald, H. Hirsemann, S. Jack, R. Klanner, A. Klyuev, H. Krueger, S. Lange, A. Marras, A. Mozzanica, R. Seungyu, B. Schmitt, J. Schwandt, I. Sheviakov, X. Shi, S. Smoljanin, U. Trunk, Q. Xia, J. Zhang, M. Zimmer

11:45 Imaging capabilities of X-ray free-electron lasers
Pablo Villanueva-Perez, B. Pedrini, R. Mokso, M. Guizar-Sicairos, F. Arcadu, and M. Stampanoni

Fixed target approach to time-resolved measurements on protein crystals at Free Electron Lasers

Nadia Opara[1,2,3*], Thomas Braun[2,3], Henning Stahlberg[2,3], Mikako Makita[1], Christian David[1], Celestino Padeste[1,3]

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Free Electron Lasers are most promising facilities for measurements of ultrafast dynamics in protein crystals [1,2]. Their ultrashort and intense X-ray pulses allow tracing fast phenomena occurring in molecules, including structural changes such as an isomerization (fs-ps), or reactions in the protein photocycle (μs-ms).

Interaction of X-rays with matter induces many processes like breaking of chemical bonds, damage induced by free radicals, as well as crystal lattice deformation in absence of further chemical damage, "melting" or Coulomb explosion.

Here, we present the *in situ* growth of protein crystals on silicon chips used as the sample delivery system for a dynamic study of the radiation damage in femtosecond range tested by means of the X-ray optics setup in the delay line geometry [3].

The microfabricated solid supports with multi-well arrays of ultrathin silicon nitride windows allow direct growth of protein crystals of the required size in nanoliter volume wells. The developed system is suitable also for crystal growth under different conditions (screening experiments).

Enclosure with analogue lids sealed with double-sided adhesion tape forms watertight chambers, which prevent fragile crystals from evaporation and allow collection of high quality diffraction data from X-ray sources.

References:

[1] Neutze R., Opportunities and challenges for time-resolved studies of protein structural dynamics at X-ray free-electron lasers, Phil. Trans. R. Soc. B 369:20130318 (2014)

[2] Schlichting I., Serial femtosecond crystallography: the first five years, IUCrJ, 2, 246-255 (2015)

[3] David C. et al., Following the dynamics of matter with femtosecond precision using the X-ray streaking method, Scientific reports, 5:7644 (2015)

Single-shot & time resolved, x-ray-pump & x-ray probe method for ultrafast dynamics

M. Makita [a], I. Vartiainen [a], I. Mohacsi [a], A. Diaz [a], P. Juranic [a], A. Meents [b], C. Milne [a], A. Mozzanica [a], N. Opara [a], C. Padeste [a], V. Panneels [a], M. Sikorski [c], S. Song [c], P. Willmott [a], L. Vera [d] and C. David [a]

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The ultrashort and intense X-ray pulse generation at many FEL facilities has opened up new possibilities to investigate sub-pulse length dynamics in time resolved manner. One of the conventionally used 'time resolving' strategies is called pump-probe method, where a single probe beam follows a pump beam at a fixed delay time. While this method has proven to be successful in many cases, it also suffers with fundamental restrictions such as data consistency, time resolution, and the applicability to the pumping dynamics. Here I present the method and results of x-ray-pump & x-ray-probe experiment using a unique diffraction grating-based setup, based on the previous experimental design [1] – a method that allows one to record the full dynamics of an X-ray pumped ultrafast phenomena, in femtosecond time resolution, and in single-shot manner.

I will present the results obtained from both organic and inorganic crystals, performed at LCLS, SLAC – a preliminary results of 9-10 consecutive time-information within 350 fs from the pump incidence, from single shots. This short probing time steps were achieved with x-ray energy of 5keV and the pulse duration of 30fs. The following key attributes will be highlighted: Firstly, the grating non-invasiveness and its alignment tolerances to the incoming x-rays, resulting in conserved optical qualities between the diffracted and the transmitted beams. Secondly, the absence of timing jitters between the diffracted beams, allowing for accurate probe timings within femtosecond tolerances. Finally, the capability of the setup to obtain diffraction signals from different pumping dynamics, leading to potential new insights.

References

[1] C.David et al., Sci. Rep 07644, DOI 10.1038, (2015)

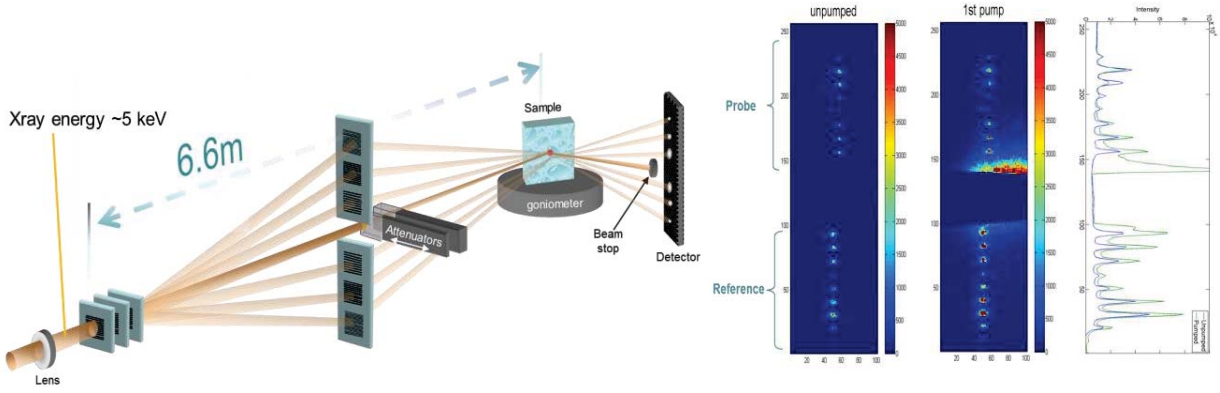

Figure: [Left] Schematic drawing of the experiment setup. The incoming x-ray beam is split by stacks of gratings, which will then be re-diffracted onto the sample by the gratings downstream, allowing each of the beams to overlap at the pumped are after controlled delay times.
[Right] Raw images of the diffracted probing beams from Bismuth crystal. Unpumped (left), pumped (centre) and projection of the two shots (right), where blue and green lines are unpumped and pumped shots, respectively.

AGIPD: A High Frame Rate Detector for the European XFEL

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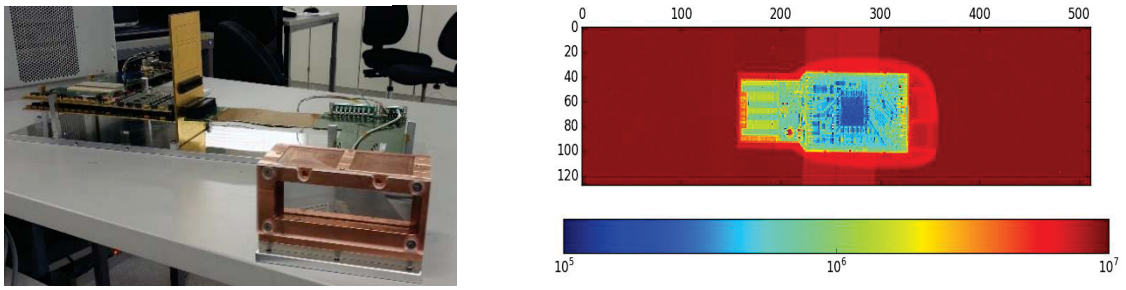
The AGIPD (adaptive gain integrating pixel detector) detector [1][2] is a high frame rate (4.5 MHz) and high dynamic range (up to 10^4 x 12.4 keV photons) detector with single photon resolution (down to 4 keV taking 5 σ as limit and lowest noise settings) developed for the European XFEL (Eu-XFEL) [3]. The full scale chip (AGIPD 1.0, see figure 1) is 64 x 64 pixels and each pixel has a size of 200 x 200 µm^2. Each pixel can store up to 352 images at a rate of 4.5 MHz (corresponding to 220 ns). In this talk the results of a detailed characterization of the AGIPD 1.0 chip showing the performance of the ASIC in terms of gain, noise, speed, dynamic range and nonlinearity will be presented. Moreover an overview of the single module assembly (see figure 2 a) and b) for a picture of the AGIPD module setup and a X-ray picture of an usb stick taken with the single AGIPD module assembly) and the 1M system will be given.

Figure 1 Layout of the AGIPD 1.0 single chip assembly. The active area and periphery (biasing blocks and command based interface) regions are marked.



a) b)

Figure 2 a) AGIPD single module setup. b) Xray image of an USB Stick done with a full working module system. The image is both gain and dark field corrected.

[1] X. Shi et al., Challenges in chip design for the AGIPD detector, Nucl. Instr. and Meth. A, 624(2):387-39, 2010.

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Imaging capabilities of X-ray free-electron lasers

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The resolution of conventional coherent X-ray microscopy techniques at synchrotrons is limited by the radiation damage and was claimed to be 10 nm for biological material [1]. Alternatively free-electron lasers (FEL) experiments can overcome this limit using ultraintense and ultrashort pulses [2], thus the resolution is limited by the the number of photons available in a FEL pulse as the sample is destroyed after each pulse. During this presentation we will aim to shed light on the imaging capabilities of free-electron lasers compared to synchrotrons and we will introduce an imaging setup capable to access 3-D information for single-shot experiments.

First, we will present the signal-to-noise criterion introduced in [3], based on a Gaussian scatterer model, which predicts whether a feature of a given size and scattering strength placed inside a larger object, can be retrieved with two common X-ray imaging techniques: a) projection microscopy (PM) in real space and b) coherent diffraction imaging (CDI) in Fourier space. Our criterion, validated quantitatively through simulations, predicts that PM technique requires less photons per unit of area (fluence) than CDI. We will also describe how to use this criterion to design optimized imaging experiments and feasibility studies at FEL and synchrotron facilities.

Standard single-shot imaging approaches at FELs only access two-dimensional information as the sample is destroyed after each pulse. We propose an experimental setup for the hard X-ray regime which permits the simultaneous acquisition of multiple projections from the same specimen, similar to the proposed idea for soft X-rays in Ref. [4], allowing for the first time to access 3-D information for single shot experiments. This setup illuminates the sample simultaneously with different diffracted beams generated from a single coherent incoming beam using a single crystal as a beam splitter, as depicted in Fig. 1. We provide an experimental proof-of-principle of this concept at a synchrotron source in both tomographic and coherent diffraction imaging geometries. For the latter, implementation at X-ray free-electron laser is straight forward.

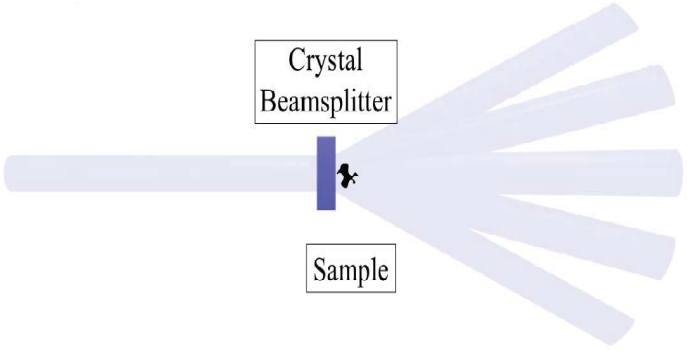

Fig. 1: Experimental setup sketch where the sample is illuminated simultaneously by all the generated beams after crystal beam splitter.

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