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Book of Abstracts





PhotonDiag 2020

5th FELs OF EUROPE Conference on FEL Photon Diagnostics, Instrumentation and Beamline Design

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Welcome

Dear PhotonDiag 2020 conference participants,

This year's organisation of the conference on photon diagnostics and beam transport has been as large a challenge as the subject matter that it addresses. With the Covid-19 pandemic bringing the world to a virtual halt and changing the way people and scientists are forced to interact and communicate with each other, we found ourselves navigating through a world of restrictions, less personal contact, and a global shift to virtual meetings, discussions, and even conferences.

Despite the shifts in the venue and organisation, and uncertainties until the early summer about how and if the conference would take place, the great support and response from the conference participants has shown that even with these troubling developments, scientists around the world are able and willing to adapt and overcome the challenges set before them and make things work. It is in that spirit that we are glad to note that this conference has broken new records in registered participants, with over 220 people signing up, and over 50 contributions submitted. We have attempted to create a program where everyone can talk, no matter where they are in the world, while also allowing the flexibility to look at individual talks and posters in your time zone without having to sacrifice sleep. Some things, like coffee break discussions and lunches with colleagues are, unfortunately, not possible in the current environment, but we have done our best to bring the online format as close as possible to an in-person conference.

The scientific contributions for this year's PhotonDiag 2020 are just as good and more numerous than those of previous conferences, and we hope that you find the experience enjoyable and educational. It is our hope that this conference is remembered for a community successfully coming together despite the conditions, and that the next conference, in two years' time, no longer has to deal with the reality of a pandemic. I wish you all an enjoyable experience!

Pavle Juranić

Chair of the PhotonDiag 2020 scientific program committee

Organisation

Programme Committee

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Industrial Partners

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Programme

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	Temporal Diagnostics I		Christian Erny		10:40-11:50
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		14	Jan Grünert	Status of the EuXFEL photon diagnostics	15:30-15:50
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		77	Job Beckers	New Detectors for Photon Diagnostics	15:00-15:30
		48	Stefan Droste	High-sensitivity Femtosecond X-ray Optical Cross-Correlator for Next Generation Free-Electron Lasers	15:30-15:50
		13	Tim van Driel	The new ePix10k megapixel hard x-ray area detector at the LCLS	15:50-16:10
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	New developments in photon diagnostics and optics II		Benedikt Roesner		16:30-17:10
		39	Christoph Braig	Diffractive wavefront correction for nearly diffraction-limited soft X-ray spectroscopy	16:30-16:50
		60	Haoyuan Li	Design of an amplitude-splitting hard x-ray delay line with sub-nanoradian stability	16:50-17:10

Date	Session	ID#	Author/Chair	Title	Time CET
28.10.20	Photon Diagnostics at synchrotrons		Volker Schlott		10:30-11:40
		51	Chris Bloomer	The use of online photon beam position measurements to improve synchrotron performance	10:30-11:00
		33	Claire Houghton	Modelling the effects of optical vibrations on photon beam parameters using ray-tracing software	11:00-11:20
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	Photon diagnostics require- ments for new experimental methods		Gregor Knopp		14:30-15:40
		53	Nikola Stojanovic	Probing THz driven solids by second harmonic generation	14:30-14:50
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	Scientific computing, machine learning and large data management		Derek Feichtinger		16:00-17:10
		26	Alexander Scheinker	Adaptive Feedback and Machine Learning for Tuning Complex and Time Varying Systems	16:00-16:30
		52	Konstantin Kharitonov	Application of automatic differentiation based ptychography for single-shot SASE FEL beams characterization	16:30-16:50
		21	Mei-Chih Chang	Developing Real-time Services for Large Volume Experiment-Data Analysis utilizing Supercomputing and Cloud technologies at CSCS (SELVEDAS)	16:50-17:10

Abstracts | Talks

Facility Overview 1

Monday, 26 October 2020, 09:00 - 10:20 CET

Welcome

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Facility Overview 1

Monday, 26 October 2020, 09:20-09:40 CET

Recent status of laser synchronization system at SACLA

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The precise synchronization between the optical laser and the FEL is of importance for the ultrafast pumpprobe experiments. For this purpose, two techniques have been developed at SACLA. One is arrival timing monitors for the hard and the soft X-ray FEL beamlines, which have ~4 fs temporal resolution. The other is a new synchronization system, which consists of a mode-locked oscillator combined with a balanced optical-microwave phase detector (BOM-PD). The typical arrival timing jitter of the new system is ~40 fs (RMS). In this presentation, we will report the recent status of the synchronization system at SACLA.

Photon diagnostics status at PAL-XFEL

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PAL-XFEL first started supporting regular user experiments in mid 2017, and total 6 instruments are currently operating at two hard X-ray (XSS: X-ray Scattering and Spectroscopy and NCI: Nano Crystallography and Imaging) and one soft X-ray (SSS: Soft X-ray Scattering and Spectroscopy) beamlines. The HX beamline provides more than 1011 photons/pulse in the range from 2.2 to 15 keV with maximum repetition rate of 60 Hz, and about 1012 photons/pulse in the range from 200 to 1200 eV are delivered at the SX beamline. All the way from XFEL tuning to the end of the user beamtime, photon beam diagnostics is an essential part of the beamline operation. This presentation includes overview of photon beam diagnostic devices at the PAL-XFEL to monitor intensity, position, spectrum, and arrival timing of the XFEL pulses.

Facility Overview 1

Monday, 26 October 2020, 10:00-10:20 CET

Photon diagnostic developments at the Athos and Aramis beamlines of SwissFEL

Authors: Andre Al Haddad¹; Christian David¹; Christian Erny¹; Christoph Bostedt¹; Christopher Arrell¹; Christopher Milne¹; Claudio Cirelli¹; Cristian Svetina¹; Eduard Prat Costa¹; Elia Razzoli¹; Eugenio Ferrari¹; Gregor Knopp¹; Henrik Till Lemke¹; Ivan Usov¹; Jens Konstantin Rehanek¹; Jonas Knurr¹; Kirsten Andrea Schnorr¹; Luc Patthey¹; Mathias Sander¹; Paul Beaud¹; Pavle Juranic¹; Philip Johnson¹; Rasmus Ischebeck¹; Rolf Follath¹; Roman Mankowsky¹; Serhane Zerdane¹; Simona Bettoni¹; Sven Augustin¹; Sven Reiche¹; Ulrich Hilmar Wagner¹; Wojciech Blachucki²; Yunieski Arbelo Pena¹; Yunpei Deng¹; Zhibin Sun¹

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With the first lasing of Athos (the soft X-ray branch of SwissFEL) in December 2019, SwissFEL is now operating two FELs in parallel. Whereas at the hard X-ray branch (Aramis) we are now mainly focusing on further developing the experimental infrastructure as well as setting up and performing user experiments, at Athos a constant progress of the beamline commissioning and the construction of endstations takes place.

In this talk, we will present the developments of X-ray photon diagnostic tools. We will highlight the facility achievements with specific focus given to spectral and temporal diagnostics of the ultrashort x-ray pulse that are required on the one hand to optimize the accelerator, on the other to provide optimum conditions for the user experiments scheduled at the beamlines. Finally, we will discuss our plans for future developments of these tools for both, Athos and Aramis.

Nonlinear optics for timing diagnosis at SwissFEL

Authors: Yunpei Deng¹; Xinhua Xie¹; Serhane Zerdane¹; Edwin James Divall¹; Christopher Arrell¹; Philip Johnson¹; Henrik Till Lemke¹; Roman Mankowsky¹; Christian Erny¹; Rafael Winkler¹; Claudio Cirelli¹; Christopher Milne¹; Gregor Knopp¹; Paul Beaud¹; Steven Johnson^{1,2}

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Timing jitter is a major issue in many pump-probe X-ray FEL experiments. Current implementations of single-shot timing diagnostic tools are based either on X-ray induced changes of the optical properties of solid-state materials, or on the modulation of X-ray generated photoelectron energies via strong field interactions. These methods nearly always rely on nonlinear processes to generate suitable conditions for the measurement.

One application of nonlinear optics is the generation of broadband optical radiation, so-called "white light", that can be used for broadband spectroscopic measurements or for the creation of ultrashort pulses. White light can be generated in a bulk crystal, a high-pressure gas cell, or a gas-filled hollow core fiber with an intense femtosecond laser pulse. White light generation in a bulk crystal has limited photon flux due to breakdown and multiple-filamentation issues. The filamentation in a high-pressure gas cell and hollow core fiber can provide greater flux in the super-continuum spectral range, but with higher noise. In addition, small changes in the gas pressure can cause significant time drifts which can impact usage in timing diagnostic tools. At SwissFEL, several systems have been developed for the short laser pulse and white light generation in order to achieve higher signal-to-noise ratio and temporal resolution. Nonlinear optics not only provides the light sources for the timing diagnosis of FELs, but also can be applied for the process used in timing tools. Current realizations of this concept in single-shot timing diagnostics in solid state media are all based on X-ray induced changes in the linear susceptibility. In the optical spectroscopy, however, nonlinear processes often offer an enhanced sensitivity to small perturbations and in some cases can provide nearly background-free signals.

Here we present the potential of using a prototype $\chi(2)$ process, second harmonic generation, to measure the X-ray induced changes and to explore its potential applications using for an X-ray timing diagnostic tool.

Figure 1 (a) Measured the correlation between the SHG spectrum encoding and spatial encoding. (b) and (d) present the distributions of the arrival time measured with the SHG spectral timing tool and the spatial timing tool, respectively. (c) The distributions of the difference in the retrieved arrival time between the two timing tools (blue: all signal; red: signals in the timi

Single-shot temporal characterization of SASE XUV pulses at FLASH FEL

Author: Rosen Ivanov¹

Co-authors: Ivette Bermudez Macias¹; Jia Liu²; Günter Brenner¹; Juliane Roensch-Schulenburg¹; Mikhail Yurkov¹; Stefan Düsterer¹

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We present a Terahertz (THz) field driven streak camera [1] with the capability to deliver the XUV pulse duration and the arrival time information with < 10 fs resolution for each single XUV FEL pulse at FLASH. Pulse durations between "350 fs and "10 fs (FWHM) have been measured for different FLASH FEL settings [2]. In particular the arrival time analysis showed the precision with which FLASH can be operated meanwhile. A comparison with the FEL electron bunch arrival time (BAM – beam arrival time monitor) in the FLASH linac section showed a very good correlation (< 15 fs rms). For the simulation and analysis of the streaking process, a standard classical approach was used as well as a quantum mechanical theory, based on strong field approximation. Various factors limiting the temporal resolution of the presented THz streaking setup are investigated and discussed. Special attention is paid to the long and short pulse limit. Additionally SASE (Self-amplified spontaneous emission) pulses are inherently fluctuating in various properties. The pulse resolved characterization of the XUV SASE pulses regarding pulse duration, spectral distribution and pulse energy provides a large set of data that can be used to investigate the dependencies of the different parameters. Using the measurements together with simulations we can disentangle accelerator based fluctuations from pure SASE contributions and provide more insight into the SASE process [3].

- [1] R. Ivanov, J. Liu, G. Brenner, M. Brachmanski, S. Düsterer, FLASH free-electron laser single-shot temporal diagnostic: terahertz-field-driven streaking, J. Synchrotron Rad. 25 26, 2018.
- [2] R.Ivanov et al. Single-shot temporal characterization of XUV pulses with duration from ~10 fs to ~350 fs at FLASH, J. Phys B: At. Mol. Opt, accepted, 2020.
- [3] I. Bermúdez Macias et al., Study of temporal, spectral and energy fluctuations of SASE FEL pulses, in preparation, 2020.

New concept for THz based X-ray pulse tomography

Author: Michael Gensch^{1,7}

Co-authors: Robert Carley²; Alexander Yaroslavtsev²; Jia Liu²; Loïc Le Guyader³; Laura Foglia⁴; Sergey Kovalev⁵; Andreas Scherz²; Naman Agarwal²; Jan Deinert⁵; Gabor Kurdi⁴; Riccardo Mincigrucci⁴; Emiliano Principi⁴; Tobias Kampfrath⁶

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In this contribution a new concept for deriving arrivaltime, pulse duration and potentially also the pulse energy of individual XUV/X-ray pulses is presented. The concept is based on the analysis of THz bursts generated by the XUV/X-ray pulses in a novel type of spintronic THz emitter. Note only the arrivaltime jitter but also the duration of the XUV/X-ray pulses can be derived from single-shot electro-optic measurements of the emitted THz waveforms. The potential of the concept is discussed based on first pilot experiments performed recently at the FERMI FEL.

MHz repetition rate Photon Arrival Time Monitor at the European XFEL

Author: Jia Liu¹

Co-authors: Henry Kirkwood¹; Romain Letrun¹; Marc Planas¹; Adrian Mancuso^{1,2}; Tokushi Sato¹; Jan Grünert¹

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Operation of the European X-ray Free Electron Laser (EuXFEL) since 2017 enables novel research of atomic-scale structures and ultrafast phenomena and dynamics. Exploiting the unprecedented high FEL peak brilliance, X-ray induced dynamics can be observed by applying X-ray pump - optical probe schemes. Typically, the timing of pulses from two independent sources can only be controlled down to the level of naturally occurring timing jitter, which limits the temporal resolution of pump and probe experiments. This unsurprisingly calls for a photon arrival time diagnostics tool to precisely determine the timing jitter and to sort and tag the experimental data. In this contribution, we describe the design of a very compact Photon Arrival time Monitor (PAM) [1] and its commissioning results at the SPB/SFX instrument [2], located at the SASE1 hard X-ray beamline at EuXFEL. This pulse-resolved measurement of timing jitter inside pulse trains with up to MHz repetition rates, together with the determination of inter-train jitter across the 10 Hz pulse trains, represents an important step towards realizing ultrafast experiments[3,4].

References:

- [1] J. Liu et al., "Technical Design Report: Photon Arrival Time Monitor (PAM) at the European XFEL," DOI: 10.22003/XFEL.EU-TR-2017-002 (2017).
- [2] A. P. Mancuso, et al., "The Single Particles, Clusters and Biomolecules and Serial Femtosecond Crystallography instrument of the European XFEL: initial installation," J. Synchrotron Radiat. 26, 660 (2019).
- [3] H. J. Kirkwood et al., "Initial observations of the femtosecond timing jitter at the European XFEL," Opt. Lett. 44, 1650 (2019).
- [4] T. sato et al., "Femtosecond timing synchronisation at megahertz repetition rates for an X-ray Free-Electron laser," Optica 7, 716 (2020).

Post-undulator time-resolved diagnostics of electron and photon beams at SwissFEL with a passive structure.

Authors: Alexander Malyzhenkov¹; Philipp Dijkstal¹; Paolo Craievich¹; Sven Reiche¹; Pavle Juranic¹; Eduard Prat Costa¹

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SwissFEL is a hard X-ray free-electron laser (FEL) facility operating at the Paul Scherrer Institute in Switzerland. We recently installed a passive corrugated structure after the undulator beamline of SwissFEL. The transverse wakefields generated by the electron beam traveling through such a device can be employed to measure the time properties of the electrons. Compared to the standard transverse RF deflector approach, the method is more cost-effective, less sensitive to arrival-time jitter, but the reconstruction of the beam profiles becomes more complicated. A comparison of the longitudinal phase-space of the electron beam with and without lasing conditions also allows reconstructing the time-resolved properties of the produced hard X-ray radiation. We present simulations studies and first experimental results of this new method at SwissFEL.

Temporal Diagnostics 2

14:10-14:30 CET

Measurement of transient optical phase as a diagnostics technique for XUV pump – optical probe experiments

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Measurement of transient optical properties (reflectivity and transmissivity) is routinely performed in extreme-ultraviolet (XUV) pump – optical probe experiments. The optical properties reflect the transient state of the irradiated materials. Here we propose to extend the material diagnostics with an additional measurement of the transient phase change of the optical probe pulse. It can be recorded in parallel to other transient optical properties, enabling access to full information on the complex refractive index and the thickness of the radiation-modified material layer. The latter is essential for investigations of phase transitions progressing in XUV (and X-ray) irradiated materials. Here we report on the computational study of XUV irradiated silicon and diamond performed in [1]. It shows that the measurement of the optical phase from a probe pulse at correctly tuned pulse parameters can provide a signal strong enough to extract information on transient material properties.

The results suggest that in some cases, it is even more preferable to measure the transient phase change than other optical parameters. Such phase measurement, feasible with modern experimental setups, can then be a basis for an improved diagnostics tool for the temporal characteristics of an ultrashort XUV pulse.

[1] V. Tkachenko et al., Optics Letters Vol. 45, 33-36 (2020).

FLASH2020+: Photon diagnostics and beam transport

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The FLASH2020+ project, a major upgrade program for the high repetition rate XUV and soft X-ray free-electron laser FLASH at DESY, aims at significantly improving the FEL photon beam properties for users. Within the project, both existing FEL lines at FLASH will be equipped with fully tunable undulators capable of delivering photon pulses with variable polarization. One of the two FEL lines will be externally seeded at the full repetition rate that FLASH can provide in burst mode. The other line will exploit novel lasing concepts based on different undulator configurations. Together with an increase in electron beam energy to 1.35 GeV this will extend the wavelength range to the oxygen K- edge in the fundamental harmonic, in order to cover the important elemental resonances for energy research and the entire water window for biological questions. The planned machine upgrade and the resulting new beam properties require a substantial upgrade of the existing photon diagnostics and beam transport.

Present status, achievements, and future developments at FERMI: photon transport and diagnostics from current operations to prospec- tive low-wavelengths upgrade

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FERMI, the Italian free electron laser operating at Elettra (Trieste), has been in user operations for eight years.

During this timespan the number of beamlines and endstations has reached the project target (6), and continuous development of the machine has taken place, too. Currently, two calls for proposals are issued per year, offering users the possibility to perform experiments on both FEL undulator lines of FER-MI, covering the 100-4nm range. Of course, also the photon transport and diagnostics system (PADReS) has evolved in this years, having to face new requests in terms of several different aspects (e.g., intensity monitors, energy spectrometers, and new optics for extended/lower wave- length operation; multiplexing solutions for the efficient use of the radiation; advanced diagnostics for ultimate focusing; etc.).

A further upgrade of the entire facility is now being discussed and developed, which foresees an increase of the machine electron energy in order to decrease the achievable wavelength to values below 2nm in the fundamental laser harmonic. The goal is to reach such lower wavelengths main- taining the unique characteristics and capabilities of FERMI, which is a seeded FEL. In particular, intensity and wavelength stability, spectral purity, coherence, polarization, and TM-00 photon emis- sion mode should be guaranteed as well as the possibility to produce two-color double pulses and other exotic emission schemes. Achieving that, a new class of experiments will be possible together with the chance to extend the current experimental capabilities in so-far non-achievable wavelength regions.

Obviously, this ambitious target calls for parallel evolution of the photon transport and diagnostics system in order to be able to efficiently cover the need for online characterizing each single FEL pulse for wavelength extending to 2nm and below. The present setup will need to be upgraded in several ways, from the energy spectrometers to the intensity monitors, from beamline design to the optical mirror coatings, and so on.

The current situation, with the solutions adopted up to now, is presented, and the possible future upgrades and developments are discussed.

Status of the EuXFEL photon diagnostics

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The European XFEL facility has entered user operation in September 2017. Since that time the base- line photon diagnostics are in routine operation, delivering online monitoring of pulse energies, beam position, and transverse beam profile. More advanced diagnostics such as monitors for spec- tral and temporal properties were also commissioned in the meantime. This presentation reviews the operational diagnostics devices in the three SASE undulator beamlines, and provides details about new diagnostic capabilities such as MHz-rate spectral and temporal monitoring at hard and soft x-rays, measurements for undulator system optimization, studies of high-repetition rate effects with pulse-resolved intensity monitors, novel diamond diagnostic detectors, absolute pulse energy measurements with calorimeters and gas-based monitors, and application of photon diagnostics for special machine operation modes and studies such as hard x-ray self seeding, two-color lasing and harmonic lasing.

Facility Overview 2

15:50-16:10 CET

Status of LCLS and Future Developments

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The Linac Coherent Light Source (LCLS) began user operations in 2009 and has performed over 500 fullscale user experiments with ever-expanded operating modes/capabilities. The facility recently emerged from a long down period where new electron transport, undulators, x-ray transport sys- tems and x-ray instruments were installed. First commissioning results of these new systems will be presented as well the status of three ongoing upgrade projects: LCLS-II, LCLS-II-HE and MEC- U.

16:10-16:40 CET

FEL Prize presentation

The FELs of Europe award is given in recognition of a distinguishing contribution in the area of free electron laser photon diagnostics, photon transport, and beamline developments as well as FEL instrumentation development in its broadest sense. FEL instrumentation developments are often long term achievements, yet the work for which the team or individual is nominated must be such that a significant component of it was performed or substantial progress achieved in the last 3 years.

The talk is given by the prize winner.



Spatiotemporal diagnostics of XFEL pulses via intensity correlation techniques

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Characterizing spatiotemporal properties of XFEL pulses is of great importance not only for ana-lyzing experiments, but for giving effective feedbacks to machine operations. As simple and cost effective ways to diagnose XFEL pulses, we have developed X-ray intensity correlation techniques, such as intensity correlation measurements of fluorescence and spontaneous undulator radiation for evaluating XFEL durations [1,2] and spatial profiles of tightly focused XFEL beam [3].

In this presentation, I will talk about the concepts of these techniques and their applications to XFEL pulses from SACLA, as well as the future perspectives.

- [1] I. Inoue et al., Phys. Rev. Accel. Beams. 21, 080704 (2018).
- [2] I. Inoue et al., J. Synchrotron Rad. 26, 2050 (2019).
- [3] N. Nakamura et al., submitted.

New Development in Photon Diagnostics and Optics 1

09:30-09:50 CET

Newly designed radiometer for synchrotron radiation and free- electron laser in high power range

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We designed a new radiometer to measure the absolute power of synchrotron radiation and free- electron laser in the wavelength range from the extreme-ultraviolet (EUV) to x-rays. The target measurable power range is from 1 mW to 1 W, which exceeds that of our former radiometer (a compact radiometer) of 0.01 mW to 150 mW. The new radiometer is directly mounted on a vacuum flange cooled with a fan, and can operate at room temperature or above (around 310 K). The mea- surement principle of the radiometer is based on a temperature measurement of an absorber, which is a component of the radiometer. The absorber is a cavity type and consists of a tungsten plate and a copper cylinder. The absorptance is higher than 99.5% for photon beams in the wavelength range from EUV to x-ray (20 eV to 60 keV); therefore, a temperature change in the absorber relates to the power of an incident photon beam. The absolute power can be evaluated from a electrical heating power applied to a heater on the absorber, namely a dynamic electrical substitution technique. We have completed the construction of the radiometer and plan to finish checking the performance of the radiometer using an electrical heating by the end of this year.

Multi-Focus Off-Axis Zone Plates for Experiments at X-Ray Free Electron Lasers

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1. General information

X-ray free electron lasers (XFELs) pave the way towards new and highly exciting experiments in the fields of X-ray imaging and spectroscopy [1,2]. They allow accessing ultrafast and non-linear processes on the nanoscale. However, the stochastic nature of the lasing process causes strong shot-to-shot fluctuations in intensity and spectral composition, which represents a challenge for many experiments in terms of signal normalization. Thus, accurate detection schemes with high correlation between the signal and a reference beam are necessary for normalization purposes to ensure good data quality in experiments that rely on the use of multiple pulses from an XFEL, such as spectroscopy and pump-probe experiments.

2. Methodology

For addressing this challenge, we have designed a new type of X-ray optic that combines the beam splitting functionality of a transmission grating with an off-axis zone plate [3]. This design not only overcomes the disadvantages of two individual optical elements, but introduces the beam splitter as a perfect phase grating, which can be implemented in a defined way to adjust the beam splitting efficiencies for certain diffraction orders precisely.

The grating can be added in two ways either by inverting the zone structure with a certain duty cycle or by shifting the zone structure by a certain factor.

3. Results

We characterized such multi-focus zone plate optics at the SIM beamline at the SLS and they enabled us to conduct the first user experiment at the Spectroscopy and Coherent Scattering beamline at the European XFEL. Here, the overlaid inversion grating generated two intense spots in the focal plane, where one interacted with the sample whereas the other one was used as a reference. In this way, we were able to measure an X-ray absorption spectrum from Ni and NiO thin films at different fluence levels with precise normalization on a shot-to-shot basis. The normalized spectrum showed a clear signal over noise improvement. These results demonstrate the capabilities of such compound optics to enable advanced experiments at XFELs.

Acknowledgements

We would like to thank everyone involved in the open community proposals No. 2161 and No. 2170 at the European XFEL. This work received funding from the EU-H2020 under grant agreement No. 701647 and No. 654360 NFFA-Europe.

References

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Resolving spectro-temporal dynamics with all-XUV-optical FEL transient absorption spectroscopy

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Extreme ultraviolet (XUV) and x-ray free-electron lasers (FELs), delivering intense ultrashort pulses in the femtosecond regime and even below, create new opportunities for site-specific light-matter interaction, and eventually to control the intrinsic quantum dynamics of a system with atomic scale resolution. Using visible lasers, the technique of ultrafast transient absorption spectroscopy and related multidimensional spectroscopies, which elegantly combine both high spectral and temporal resolution through multi-pulse sequences, are now routinely used both for understanding and con- trolling photochemical reactions, however typically coupling only to the valence shell of the binding electrons and the intramolecular vibrational degrees of freedom, which is directly linked to the low photon energies being used (from infrared to visible and ultraviolet).

In this talk I will give an overview of our recent efforts to perform all-XUV-optical transient absorp- tion spectroscopy of gas-phase atoms and molecules [1-3]. Hereby we have proven sensitivity to element-specific spectral signatures identifying resonant electronic transitions in the XUV and how they are modified (both Stark shifts and line-shape asymmetry changes) due to the presence of the strong XUV free-electron laser electric field. Furthermore, transient spectro-temporal signatures could be extracted from the data, with a timescale below 3 femtoseconds, and understood through nonlinear interaction of pump and probe beams in the target medium, revealing direct sensitivity to the coherence properties of the FEL pulses. This can be regarded as a precursor to coherent multidi- mensional spectroscopy in the XUV spectral range.

An important ingredient for such measurements is a profound knowledge of the spectro-temporal properties of the employed FEL pulses. In our experiments we utilize the quasi-instantaneous non- resonant ionization dynamics of neon atoms in response to an FEL pump pulse as an ultrafast optical switch to modulate the XUV absorption properties of our gas target with timing precision below one femtosecond. Thereby, upon spectrally resolving the FEL probe transmission spectrum with a grating-based spectrometer, we are directly sensitive to the average chirp of the FEL probe pulses, revealing a pronounced positive chirp of about 30 fs² for the particular FEL machine settings [4]. Most importantly this is a direct spectro-temporal measurement, tracking the transmitted FEL pho- ton energy spectrum as a function of pump-probe delay. No additional external laser pulses, which are typically challenging to synchronize at the precision level of a femtosecond, are needed for this all-XUV-optical scheme. Besides the importance of in-situ measuring such spectro-temporal pulse properties in transient-absorption and multidimensional-spectroscopy experiments, this new char- acterization method may also develop into a useful tool in general, extending the diagnostics toolbox of FEL pulses.

I gratefully acknowledge the fruitful collaborations [1-4] during our previous measurement cam- paigns at the Free-Electron-Laser in Hamburg (FLASH) at DESY.

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High-Resolution Pulse-to-Pulse Spectral Monitoring for SwissFel

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The spectrum of SASE XFEL sources exhibits strong variations pulse-to-pulse. As a consequence, XFEL-driven experiments, XFEL optimization or "new-modes" development rely on X-ray spectrometers functioning on a shot-to-shot basis.

We will discuss the potentiality of the setup used at SwissFEL, as well as results obtained during its commissioning.

Several arrangements of transmission gratings, e.g. having a pitch of 100 nm, and bent crystals (e.g. Si(220)) with various bending radii (e.g. between 75-200 mm) allowed measuring the SASE spectrum with high resolution, e.g. about 0.4 eV (FWHM) at 7.1 keV was achieved without gratings. Possible "dependencies" with the FEL profile or bent crystals alignment, as well as "dispersive" XAS measurements will be presented.

Flat field soft X-ray spectrometer based on reflection zone plates

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The reflection zone plate (RZP), as a wavelength-dispersive optical element, has been successfully used in several designs of femtosecond (fs) spectrometers and monochromators for soft X-rays [1]. While demonstrating its evident advantages in comparison with conventional VLS gratings, like a high resolving power at the design energy and an excellent signal-to-noise ratio, RZPs on planar substrates suffer from a narrow energy range in parallel spectral registration, limiting the applications of this type of optic. Recent developments in theory, technology, and metrology of RZPs make it possible to fabricate RZPs on spherical substrates with a small radius of curvature down to 2 m.

In this work, we report on first results obtained with newly designed high-resolution soft X-ray fluorescence spectrometer, based on RZPs, which were fabricated on a spherical substrate. High resolution flat field spectra within about \pm 50 % around the design energies were measured in the interval from 150 eV to 750 eV, using only two RZPs: The 1st RZP with its design energy of 277 eV covers the band (150 – 550) eV and the 2nd RZP with a design energy of 460 eV covers the band (350 – 750) eV, where the upper bound to this energy range is defined by the Ni coating of the RZPs. The absolute diffraction efficiency reaches 25 % and 20 % at the design energies 277 eV and 460 eV, respectively. The energy resolving power E/ E exceeds 2000 in the entire energy range. To compensate the slope error of the substrate, an algorithm for diffractive wavefront correction [2] was used in the calculation of the groove structure.

The development of theory and technology for RZPs on figured substrates opens new possibilities for a considerable improvement of the instrumental performance in soft X-ray spectroscopy, pushing forward the frontiers in time, resolving power and efficiency of dispersive optical elements. Successful results of tests enabled NOB GmbH to start customer-oriented production of RZPs on spherical substrates for spectroscopic applications.

This work was supported by the project REFLEX, Berlin Program ProFiT co-financed by the European Regional Development Fund (ERDF) and project NeuGaR, partly financed by the Federal Ministry for Economic Affairs and Energy.

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FEL beam diagnostics and source metrology

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After the first decade of operability, the strong quest for results around the Free Electron Laser (FEL) facilities has been positively filled, giving the opportunity to make one step back from the sample- level and to focus on subtle, still open topics concerning the FEL source metrology and coherence characterization. Because of the complexity of the emission process, important parameters such as the effective source position and dimension may be a-priori not known and depend on the required machine optimization, or can be adjusted to meet the experiment needs. The idea of using wavefront sensing techniques, usually employed for optics tuning, is captivating because of their shot-to-shot operability and accuracy, which make them robust and suitable as a feedback for FEL machine-tuning operations. Here we review the results of source metrology measurements at the FERMI seeded- FEL performed at distinct machine configurations, by means of Hartmann wavefront sensing. The effects of the transport optics, which may introduce curvature alterations, are discussed as well, with particular attention to the case in which shot-to-shot properties of the source are investigated (e.g. source position fluctuations) and local curvature effects of the optics come into play.

Coherence, Profile and Position Measurements

14:00-14:20 CET

Autocorrelation measurement of the FEL coherence and pulse length using a magnetic delaying chicane in the undulator beamline

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A delay of the electron beam with respect to the FEL radiation field can be used for auto-correlation measurements since the phase is imprinted both in the radiation field as well as the microbunching.

As long as the delay is within the coherence length of the SASE spikes there is interference, resulting in a modulation of the output power, similar to a phase shifter. For longer delays the bunching is overlapped with a different spike, which shows in average no dependence on the delay due to the arbitrary phase relation between the bunching and the radiation of the other spike. Even further delays will separate the radiation field from the electron bunch reducing further the output power of the FEL signal, since the FEL starts from the spontaneous radiation again. Therefore a scan of the delay can give information on both the coherence length and the FEL pulse length with a resolution on the scale of the radiation wavelength. We present simulation examples for SwissFEL that show the validity and feasibility of the method.

Towards Pulse-by-pulse XFEL Beam Measurement

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Characterization of XFEL beams can be challenging, requiring the use of several different types of detectors to measure beam properties. Sensors fabricated using electronic grade single crystal diamond have been shown to have rapid response and enable measurement of signals over a wide dynamic range for synchrotron beams. To study the utility for measurement of XFEL beams, flux linearity and temporal response measurements were performed at the SwissFEL Bernina station with two such devices through a collaboration formed during PhotonDiag2018. Comparisons were made with synchrotron beam measurements (flux linearity, spatial uniformity and temporal response) performed at NSLS-II using the same detectors prior to and subsequent to FEL beam testing. The results indicate a relationship between flux linearity and temporal response, which may provide guidance for improved detector design. Development of these monitors holds promise for enabling measurement of the intensity (and potentially also position) of single XFEL pulses over a significant dynamic range.

New Detectors for Photon Diagnostics

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Diagnosing ionizing radiation has been subject of research as long as applications in this field exist. Many techniques to reveal temporal and spatial information about a beam of ionizing photons are intrusive. To minimize this intrusiveness, plasma could be a suitable intermediate state for potential diagnostics to be developed. The in this contribution elaborated novel diagnostic is based on using a very small fraction of the radiation to partially photo-ionize a low pressure background gas. As a result, this background gas is turned into a plasma which can be – based on its permittivity - further characterized by traditional plasma diagnostics. For this characterization, the beam of photons is sent through a cylindrical metal pillbox cavity filled with a sensing gas at low pressure. The free electrons in the plasma induced in this cavity are probed by having them interacting with a standing electromagnetic wave in the microwave frequency range (a few GHz). Tracking temporally resolved the resonance frequency of this standing wave reveals information about the radiation beam in terms of power, alignment and stability. This contribution elaborates on the physical principles of the method and highlights the newest developments towards in-line beam monitoring.

High-sensitivity Femtosecond X-ray Optical Cross-Correlator for Next Generation Free-Electron Lasers

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The large-scale nature of free-electron lasers (FELs) often precludes control over various noise sources affecting the arrival time of the X-ray pulses. To achieve high temporal resolution (<100 fs) in laser pump/X-ray probe experiments, an arrival time monitor (ATM), such as an X-ray/optical crosscorrelator, is implemented. Typically, an X-ray-induced change of the optical properties of a target is used to derive the arrival time of the X-rays relative to the optical pump laser. These ATMs often require soft X-ray fluence levels of >1 mJ/cm2. The next generation of high-repetition FELs, such as the European XFEL and the Linac Coherent Light Source II (LCLS-II), take advantage of superconducting accelerators to enable repetition rates of up to 1 MHz. As a result of the increase in repetition rate, the energy per X-ray pulse will decrease. The X-ray fluences required by current ATMs cannot be achieved with high repetition rate FELs or when using few and sub-fs X-ray pulses. The novel ATM scheme described here solves this problem by achieving unprecedented sensitivity to soft X-rays.

Current ATM designs at FELs use a portion of the pump laser beam at a wavelength of 800 nm or white light in the visible range to probe an X-ray induced material change. However, state-of-the-art optical timing distribution systems operate at a wavelength of 1550 nm and are an enabling technology for sub-10-fs timing jitter between X-rays and pump lasers. Therefore, the ATM presented here cross-correlates X-rays and 1550 nm optical pulses to pave the way to directly derive the X-ray timing jitter measured with respect to an optical master oscillator.

The X-ray/optical cross-correlator is based on a time-to-space mapping geometry and takes advantage of 1) a specially designed multi-layer target, and 2) an interferometric detection scheme. The sample used here is made of a thin film of germanium, sputtered on a 2 μ m thick diamond layer grown by Chemical Vapor Deposition (CVD) onto a silicon dioxide layer on top of a silicon substrate. This multi-layer structure shows optical interference effects (etalon) in reflectivity, which are designed to exhibit a node in the reflection spectrum around 1550 nm. The X-ray induced changes to the sample shift the center wavelength of this node leading to dramatic amplitude and phase changes of the reflected 1550 nm light, allowing to detect extremely weak X-rays when combined with an interferometric detection scheme.

The X-ray/optical cross-correlator described here has been tested during an experiment on the LCLS soft X-ray beamline at an X-ray photon energy of 530 eV and a pulse repetition rate of 120 Hz. We achieved a ~100-fold increase in the relative signal change as compared to previously demonstrated techniques. The resolution of the timing measurement is estimated to 2.8 fs (rms), making this crosscorrelator well suited for sub-10-fs timing jitter operations at LCLS and other FELs.

The new ePix10k megapixel hard x-ray area detector at the LCLS

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The ePix10k2M is a new large area detector specifically developed for X-ray Free Electron Laser applications. The hybrid pixel detector was developed at SLAC to provide a hard X-ray area detector with a high dynamic range, running at the 120 Hz repetition rate of the Linac Coherent Light Source (LCLS). The detector has a dynamic range from single photon counting up to 10.000 photons/pixel/pulse at 8keV. The high dynamic range is achieved with 3 distinct gain settings (Low, Medium, High) as well as two autoranging modes (high-to-low and medium-to-low).

Here we evaluate the detector performance in comparison with the previously deployed CSPAD. The external dimensions of the two detectors are similar, making the upgrade from CSPAD to ePix10k straightforward for most setups at LCLS, with the sPix10k improving on experimental performance. The main detector during an experiment, such as the large area ePix10k, is used for primary signal detection. However, this detector is also often used for normalization and for diagnostics of the experimental setup, it is therefore crucial that these multi-purpose detectors are well understood and calibrated to facilitate the best scientific output of the limited XFEL beamtime.

Here we present the first measurements on this new ePix10k detector and evaluate the performance under typical XFEL conditions during an LCLS x-ray diffuse scattering experiment measuring the 9.5 keV x-ray photons scattered from a thin liquid jet.

The SLAC developed ePix cameras all utilize a similar platform and are designed to provide an upgrade path for future high repetition rate XFELs such as LCLS-II and LCLS-II-HE.

Diffractive wavefront correction for nearly diffractionlimited soft X-ray spectroscopy

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We report on the development of an accurate and flexible concept to compensate for two-dimensional slope errors of mirrors or reflective gratings as used in wavelength-dispersive soft X-ray spectroscopy.

Our approach enables an ultra-high spectral resolving power with low-cost optical components [1]. Modern soft X-ray spectrometers often use a toroidal mirror in combination with a variable line space grating. However, the curved mirror / grating substrate typically suffers from figure errors, leading to an aberrated wavefront. In close analogy to computer-generated holograms, that phase distortions are converted into a customized groove structure of the grating, the so-called "diffractive wavefront corrector". Either the probed height profile (ex situ) of the substrate or deterministic phase retrieval from the intensity distribution along the propagating X-ray beam (in situ) may be used to derive the phase [2].

We consider popular instrumental configurations, like the "Hettrick-Underwood" setup or the compact "all-in-one" device, where the grating is inscribed in the curved mirror, and apply an appropriate variety of experimental procedures and the associated computational framework to evaluate the optical path difference (OPD). This function yields the grating vector field of the DWC as its gradient.

Characteristic, slightly aperiodic and – in general – asymmetric groove structures are obtained, which differ from the regular line density distribution of, e.g., analogous reflection zone plates on a scale of $\tilde{\mu}m$. Lamellar gratings of that kind may be fabricated conveniently by direct laser writing, especially in their three-dimensional (3D) implementation on a curved substrate.

Ray tracing simulations of our DWC spectrometers predict an energy resolution which is pushed close to the diffraction limit around the design energy, while the photon flux of the initial, uncorrected instrument can be maintained.

This work is funded by the Bundesministerium für Wirtschaft und Energie within the project "NeuGaR" (ZF4302303SY8).

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Design of an amplitude-splitting hard x-ray delay line with sub- nanoradian stability

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Measurements of the dynamics of a material on the fs-to-ns temporal scale and atomic length scale provide essential information to guide our understanding of disordered materials. Split-pulse x-ray photon correlation spectroscopy (spXPCS) was recognized early in the development of the Linac Coherent Light Source as a technique that could possibly provide critical measurements of these dynamics. To conduct spXPCS measurements at fs-to-ns scale, two identical x-ray pulses are delivered to the same spot on the sample, along the same direction, with a tunable time separation over the

time scale of interest. This time regime is currently beyond the capability of the two-pulse accelerator based machine operation modes at free electron laser (FEL) facilities, and was expected to be reached with the x-ray analog of a visible optical split-delay instrument.

Such x-ray optical systems, usually referred to as x-ray split-delay optics, have seen many iterations since the first x-ray FEL facility became operational. Thin Bragg crystals were initially favored and explored as the beam splitter. However, residual strain and beam-induced thermal-mechanical issues in the thin crystals have prevented their effective use for XPCS experiments so far. Later, wave-front splitting designs adopted edge-polished silicon crystals for dividing the wave-front into two halves, and demonstrated stable and routine delivery of two microfocused x-ray spots to the sample with promising stability for pump probe experiments. However, a non-negligible crossing angle between the two beams, as a result of the wavefront splitting mechanism, poses a serious challenge for realizing visibility spectroscopy measurements. Wave-front splitting also makes the output beam properties sensitive to beam pointing jitters, and this degrades the effective spatial overlap.

Sun et al. proposed an all channel-cut split-delay design that demonstrated superb pointing stability which is a critical requirement for two-pulse x-ray experiments. This design, however, suffered from the pulse front tilt and photon energy dispersion due to the use of asymmetric reflections. Here we present a modified version of the all channel-cut split-delay system design. It realizes amplitude-splitting and the earlier technical difficulties are expected to be overcome. In this new design, a pair

of ϖ -phase-shift transmission gratings are introduced as the amplitude splitter and recombiner. An additional pair of asymmetric channel-cuts are introduced in the delayed branch to eliminate the dispersion and pulse front tilt. A performance analysis of wave propagation through a prototype model using dynamical diffraction theory revealed that sub-nanoradian relative pointing stability during a delay scan can be achieved.

We believe that this new design, once realized, will represent a significant step towards realizing splitpulse x-ray photon correlation spectroscopy at FEL facilities investigating ultrafast equilibrium dynamics of disordered matter.

The use of online photon beam position measurements to improve synchrotron performance

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For users to take advantage of the low emittance and high coherence photon beams produced at synchrotron light sources, sub-micron source-point stability is desired over timescales from milliseconds to hours. However, it is insufficient to only monitor the source electron beam; the X-ray beam itself must be monitored and, where required, included in feedback loops to meet the stringent requirements of beamlines and users. Variations in the photon flux intensity or profile can severely reduce the quality of the X-ray data collected, thus it is important to make accurate, online, and preferably non-destructive measurements of the photon beam itself. The use of photon beam diagnostics at synchrotrons is well-established, and is an essential tool to commission, optimise, and improve the light delivered to users. This paper reviews various photon diagnostics techniques in use at different synchrotrons, and discusses how their measurements are applied to improve both machine and beamline performance.

Photon Diagnostics at Synchrotrons

11:00-11:20 CET

Modelling the effects of optical vibrations on photon beam parameters using ray-tracing software

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A method to simulate beam parameters observed at a beamline sample point in the presence of motion of optical components has been developed at Diamond Light Source. Stationary ray-tracing simulations are used to model the impact on the beam stability caused by dynamic motion of optical elements. Ray-tracing simulations using SHADOW3 in OASYS, completed over multiple iterations and stitched together, permit the modelling of a pseudo-dynamic beamline. As beamline detectors operating at higher frequencies become more common, the beam stability becomes crucial. Synchrotron ring upgrades to low emittance lattices require increased stability of beamlines in order to conserve beam brightness. By simulating the change in beam size and position an estimate of the impact certain motions have on stability is possible. The results presented in this paper focus on modelling the physical vibration of optical elements. However, the basic principle can be applied to any parameter which dynamically changes. Multiple situations can be analysed in succession without manual inputs. In this paper we describe the simulation code and present the results obtained. This method can be applied during beamline design and operation for the identification of optical elements that may introduce large errors in the beam properties at sample point.

Probing THz driven solids by second harmonic generation

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THz sources at FLASH utilize spent electron beam from an soft X-ray FEL to generate very intense (up to 150µJ), tunable frequency (1-300THz) and ultrafast narrow-band (~10%) THz pulses, which are naturally synchronized to soft X-ray pulses. This unique combination allows for wide range of element specific pump-probe experiments in physics, material science and biology.

THz pulses are completely temporally characterized by a jitter corrected Electro-Optic-Sampling(EOS) THz pulse characterization over a broad spectral range (0.1 - 8 THz).

In this work we report on the installation of new probing technique that enables study changes of material symmetry, by second harmonic generation of the probing fs-laser. Instrument allows detection of 2nd harmonic both in transmission and reflection, allowing probing of bulk and surface effects and matching THz excitation depth, e.g. at and off of absorption resonances. Instrument employs arrival time jitter correction and has temporal resolution better than 10fs.

Photon Diagnostics Requirements for new Experimental Methods

14:50-15:20 CET

Characterizing isolated attosecond pulses with angular streaking

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The development of isolated attosecond pulses (IAP) with the free-electron laser at LCLS called for a high-resolution, single-shot diagnostic method. In this talk I will discuss the use of angular streaking to characterize IAPs. An IAP with sufficiently high photon energy will ionize an atomic system to produce photoelectrons. In the presence of the IR field, the energy of the ionized photoelectron will be modulated, or streaked, depending on the phase of the IR laser field at the time of ionization. Through the streaking interaction, information about the temporal profile of the IAP will be encoded in the energy (and momentum) distribution of the emitted photoelectrons. Using a circularly polarized streaking laser, the temporal profile of the electron wavepacket is encoded in the angular distribution of streaked photoelectrons.

Multi Resolution Cookiebox Optimized for Future Free Electron Laser Experiments - MRCOFFEE

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A major upgrade of the LCLS facility, the LCLS-II project, is now underway. LCLS-II is being developed as a high-repetition rate X-ray laser with two simultaneously operating, independently tunable FELs. It features a 4 GeV continuous wave superconducting linac that is capable of producing uniformly spaced (or programmable) ultrafast X-ray laser pulses at a repetition rate up to 1 MHz spanning the energy range from 0.25 to 5 keV. Furthermore, the XLEAP sub-femtosecond soft X-ray pulse generation program is scalable to LCLS-II repetition rate [1].

We have designed, based on the Viefhaus et al. Cookiebook [2], an angle-resolving array of 16 electron time-of-flight spectrometers that allow wide and adjustable energy acceptance windows. By interleaving detector retardations, we enable simultaneous angle-resolved photo-electron and Auger electron spectroscopy as is required by cutting edge molecular frame spectroscopies and diffraction. The spectrometer array will be available for spectral-polarimetry measurements as well as polarization sensitive attosecond resolving temporal characterization of LCLS-II pulses. This multipolarization and multi-color spectral diagnostic/experiment endstation will have an energy resolution better than the expected seeding spectrum and the SASE spectral features.

We would like to present the next generation of high resolution electron spectroscopy endstation and FEL generated X-ray pulse diagnostic – MRCOFFEE. This talk will present the important science opportunities, new diagnostic capabilities of this newly designed TMO instrument/diagnostic.

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Adaptive Feedback and Machine Learning for Tuning Complex and Time Varying Systems

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Machine learning (ML) approaches such as neural networks (NN) and Gaussian processes (GP) are powerful tools that can learn input-output models of complex systems directly from data. Because of their strengths ML methods have been growing in popularity in all areas of science and engineering. One limitation of such methods is that if the system which generated the training data changes with time, the accuracy of the models that were learned based on that data begins to drift. Model independent feedback methods that are robustness to noise and can adapt to time varying systems exist, but their limitations include a chance of getting stuck in a local minimum if searching over a very large parameter space. By combining the ability of ML data-based methods to learn the global features of large parameter spaces with model-independent adaptive feedback, we can build an overall system that is both robust and globally optimal. At Los Alamos National Laboratory (LANL) we have begun studies of adaptive ML methods for time varying systems. Our initial results have focused on particle accelerators and their beams which are large complex systems in which both the components (hundreds of coupled magnets and RF cavities) and the beams (complex objects living in 6D (x,y,z,x',y',E) phase space) vary unpredictably with time. The time variation and complexity of accelerators results in days - weeks of hands on tuning after outages or when switching between significantly different beam setups. In this talk I will start with an overview of adaptive model-independent methods that we have developed and implemented at particle accelerator facilities around the world for automated beam tuning and accelerator optimization including the LANSCE linear accelerator at LANL, the Eu- XFEL at DESY, the AWAKE experiment at CERN, the FACET-II plasma wakefield accelerator facility at SLAC, and at the LCLS FEL at SLAC. I will then present some of the first adaptive ML results that we demonstrated at the LCLS FEL for adaptive tuning of the longitudinal phase space (time vs energy) of the LCLS electron beam and will present an overview of adaptive ML approaches. Finally I will discuss how these same principles can be applied to the experimental beam lines at accelerators which are also complex systems that require frequent and lengthy tuning.

Application of automatic differentiation based ptychography for single-shot SASE FEL beams characterization

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Wavefront sensing and characterization of the spatial and coherent properties of the Free-Electron-Lasers (FELs) radiation is vital for experiment planning, beamline optics alignment and the photon diagnostics. At the Free-electron LASer at Hamburg (FLASH), the Hartmann wavefront sensing is a typical technique used for the single-shot beam characterization. However, it is working in the assumption of the fully spatially coherent radiation and has resolution limited by mechanical components. Ptychography is another promising technique, which can provide us with high resolution complex wavefields of the FEL radiation. Ptychography is a scanning coherent diffraction imaging technique, which utilizes mutual overlap between neighboring scan positions for enforcing of the additional constraints during the reconstruction. These constraints make it robust and free of the reconstruction artifacts possible in the other CDI techniques. Ptychography allows to reconstruct complex sample function together with the complex wavefield of the illumination with diffraction limited resolution, and thus, it is frequently used for the beam characterization purposes.

Typically, ptychographical reconstruction assumes constant illumination, and can treat partially coherent illumination by usage of multimodal beam assumption. However, in this case, modal composition also should be constant for each shot, and spatial shot-to-shot fluctuations should be minimized. This conditions cannot be easily fulfilled at Self-Amplified Spontaneous Emission (SASE) FELs with their fluctuating and partially coherent beams.

In this work, we suggest to use a novel automatic differentiation (AD) based ptychographical engine which is able to perform reconstructions under these conditions. AD allows to split ptychographical algorithm into independent forward model, which can be flexibly changed, and optimization routine. This flexibility allows to adapt the forward model to the specifics of ptychographical experiments at SASE FEL and to perform the reconstructions in the assumption of multi-modal spatially fluctuating illumination, with the unique modal composition for each individual shot.

We present an AD-based ptychographical engine applicable for ptychography at FELs. With its help we were able to reconstruct complex wavefields of the FLASH2 radiation during the ptychographical measurements. Applications of AD-based ptychography to beam characterization and possibility of reconstruction of individual shots characteristics will be discussed.

Developing Real-time Services for Large Volume Experiment-Data Analysis utilizing Supercomputing and Cloud technologies at CSCS (SELVEDAS)

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Introduction

The ongoing developments in accelerators, detectors and experiment automation is leading to a rapid growth of data generated during experiments. A viable solution is utilizing suitable infrastructures that allow additional remote high performance capacity for processing and analysis of data from the experimental facilities with larger data volumes and higher processing needs. The SELVEDAS project proposes a hybrid cloud infrastructure, offering scalable and extensible services for data management and analysis to Swiss academic users by leveraging high performance computing (HPC), storage, networking as well as cloud technologies and orchestration. The on-demand services perform as a highly efficient remote data processing system providing fast feedback and analysis with the long time storage and archival of petabytes of data.

Approach

Hybrid cloud

The SELVEDAS project develops a hybrid cloud extension to the PSI infrastructure by giving access to the supercomputing resources at CSCS for experiment data analysis. The solutions rely on the easy transferability of workloads between systems comprising of HPC and cloud technologies. The architecture is data-driven (figure 1). The proposed services at CSCS are accessible through a REST- ful API, FirecREST.



On demand service

Online analysis at PSI refers to processing of data

while the scientist is using an instrument. Hence an on-demand service for advance resource reservation is implemented to realize the requirement of availability and to provide a tight feedback loop for the experiments 1. To end users, HPC resources can then be of no differences from the facility's on-site IT infrastructure resources.

Data catalog extension

Since 04/2018, CSCS and PSI jointly operate the PetaByte Archive located at CSCS. The PetaByte Archive provides user services for long term data storage and retrieval of experimental data from PSI large scale facilities. Archiving and retrieval of data is facilitated by the Data Catalogue (SciCat). The SELVEDAS project extends SciCat by integrating it with the FirecREST API and provides services for the analysis of experiment data stored in the PetaByte Archive at CSCS (figure 2).



Cross-site authentication

Authentication and authorization are based on the PSI user account and access rights. PSI client uses service accounts from CSCS for accessing FirecREST API (figure 3). This separation of responsibilities frees PSI users from needing CSCS's personal accounts, improves user scalability, and allows decentralized authentication since it's done directly by PSI clients to an OIDC server (Keycloak) in CSCS.

Performance Result

The performance evaluation is tested on the typical experiment dataset. Figure 4&5 reports results of



workflows and the job submission, one compared between two workflows with the large and small dataset, and another one compared between different GPUs for the job submission.



Conclusion

The SELVEDAS project demonstrates the feasibility of a hybrid cloud infrastructure supporting ondemand services with fast feedback analysis and analysis for archived data on the petabyte archive. The approach has been developed to provide the flexibility and extension to allow other institutions or domains to adopt similar approaches.

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Abstracts | Posters

Poster Session: 26.10.2020-28.10.2020

Poster Session

A diagnostic spectrometer for the CLARA Test Facility FEL at Daresbury Laboratory

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One of the functions for the CLARA linac at Daresbury Laboratory is a test-bed for FEL technologies. When fully constructed, the linac will have a FEL producing light in the range 100 to 400 nm. The flexibility of the linac and FEL will enable the viability of various schemes for producing improved and novel light output (e.g. single mode, frequency combs etc) to be tested.

A key need for verifying the FEL operation is to measure the spectrum of the light output. Singleshot measurement is necessary so an imaging spectrometer is required. Depending on the FEL mode, a resolving power of between 3000 and 20000 is required and a measurement range of up to 12.5% of the central wavelength.

To meet the requirements, a design using a plane grating with varied line spacing is being investigated. The design will use a variable included angle via a folding mirror to give an additional degree of freedom so that the exit beam is at a fixed angle and the central wavelength is focussed at a fixed distance. The imaging detector has to be tilted relative to the central wavelength to give optimum resolution along the image plane, but the range of tilt is not large.

The expected performance of the spectrometer is analysed analytically using the optical path function method and the results checked by ray-tracing in SHADOW.

Intensity normalization for X-ray absorption measurements at an FEL using transmission-grating beam-splitters

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X-ray absorption spectroscopy requires precise normalization of the measured absorption signal to the incident photon flux. At SASE-FELs, this incident flux fluctuates especially strongly after monochromatization. To measure absorption in transmission or reflection geometries, both incident and final flux must be measured synchronously. This poses the challenge to implement two separate but highly comparable spectral intensity measurements on the same photon pulses.

Here we demonstrate the use of a transmission grating to split the FEL beam into pairs of identical diffraction orders, thus enabling parallel measurements of two highly correlated beams on the same CCD detector. For spectroscopic measurements, a second grating is used to spectrally disperse both beams orthogonally to the beam separation on the detector.

As the spectral coherence of SASE-radiation is limited, special care must be taken to compare intensities only at exactly corresponding photon energies.

In this talk I highlight two implementations of this referencing scheme at the FL24 and PG2 beamlines at FLASH and evaluate the sensitivity to absorbance changes.

Poster Session

Characterization of the Photo-Electron Spectrometer for soft X- ray photon diagnostics at the European XFEL

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A Photo-Electron Spectrometer (PES) with 16 electron Time-Of-Flight (eTOF) drifttubes is being operated at the European XFEL for the application of pulse resolved and non-invasive spectral and polarization photon diagnostics.

Each eTOF consist of four electrode segments for retardation and focusing of photoelectrons. A Helmholtzcoil and a magnetometer are used to cancel out stray magnetic fields.

In this contribution we present, based on experimental data and computer simulations, a systematic characterization of the spectrometer performance.

The purpose is to optimize the spectral resolution and also to provide a complete map of TOF to kinetic energy calibration.

Furthermore, we quantify the impact of the Helmholtz coil to prevent loss of photoelectrons.

Realizing accurate and on-the-fly contrast determination for xray speckle visibility spectroscopy

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X-ray free electron lasers (FELs) enable the capability of probing ultrafast nano- and atomic-scale dynamics in amorphous and disordered material systems via speckle visibility spectroscopy. In the low count rate regime as is often the case, visibility is extracted via photon statistics analysis, i.e., by estimating the probabilities of multiple photons per pixel events using pixelated detectors. Given the noidealities of x-ray detectors including charge cloud sharing between pixels, pixel readout noise and gain non-uniformity, contrast extraction relying on photon assignment algorithms can be computationally demanding and often suffer from systematic errors. By simulating the response of a real-life hard x-ray detector, we first present a detailed error analysis of most frequently used algorithms, which all yield biased contrast estimations but consistent linear responses to contrast changes with similar signal to noise performance. We then demonstrate a contrast calibration procedure, where we adjust the contrast levels in the scattering by changing the diffraction volume size and determine the absolute contrast values by utilizing a detector calibration mask. The mask material is opaque to x-rays with periodic laser-machined aperture arrays aligned to detector pixel arrays, aimed at only transmitting photons without position ambiguities, e.g., center area of each detector pixel. The calibration coefficient of the evaluated algorithms can be obtained by comparing the contrasts estimation from these algorithms with the absolute values. We show that with proper calibration, the simple and computationally lightweight algorithms can be easily run on-the-fly and enable live feedback to experiments.

Generation of photoelectrons in water medium by a SASE X-ray pulse

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X-ray free-electron lasers (XFELs) emit ultra-short (femtosecond) X-ray pulses that allow to probe a target sample within time shorter than the propagation of X-ray-induced damage. The damage considered in terms of the structural change needs about 50 fs to induce observable effects and can be overcome using sub-50 fs X ray pulses. In this so called probe-before-destroy approach the much faster electronic structure change should be considered as well, as it has been shown to have a significant influence on the X-ray emission spectroscopy (XES) data 1 and may alter the X-ray diffraction (XRD) data [2,3].

This work presents simulation of energy and time distribution of photoelectrons released in water irradiated with 30 fs-short X-ray pulse of two different temporal envelopes: a spiky SASE profile and a Gaussian 4. The calculation was done within a kinetic model for 3 incident photons energies: 4, 6 and 8 keV and for typical XFEL beam parameters in the intensity domain below the sequential photoionization regime. The results show that the amount of energetic electrons may be comparable and exceeding that of the incident photons, particularly for soft X-rays. The induced electron flux may take significant part in ionization of the sample dissolved in water 1 and embedded in soft matrices. The presented results call for consideration in X-ray experiments the electron flux induced in the studied sample by the probe X-ray beam, even with ultra-short XFEL pulses.

Acknowledgements: This work was supported by the National Science Centre (Poland) under grant no. 2017/27/B/ST2/01890.

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Influence of the stochastic SASE pulses' time structure on photoionization yields via nonlinear processes

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The advent of high intensity X-ray radiation sources – the X-ray Free Electron Lasers (XFEL's) provides an opportunity for experimental investigation of the yet unexplored states of matter, as it allows nonlinear photon-matter interaction. The self-amplified spontaneous emission (SASE) mode of XFEL's provides pulses of radiation characterized by high intensity and unpredictable in terms of temporal structure. This unique property results from the stochastic nature driving the process of X-ray generation and needs to be carefully taken into consideration in the theoretical studies on nonlinear effects [1,2]. The main phenomena that may be influenced in photon-atom interaction by a stochastic pulse structure are sequential photoionization, multiphoton excitations such as twophoton absorption (TPA) and saturable absorption that may result from all of above [2–4]. Excitation of core atomic shells via multiphoton processes allows for probing electron transitions forbidden in the linear regime, governed by the special selection rules (e.g. quadrupole transition in the case of TPA).

The development of XFELs may lay foundations for new experimental techniques like two-photon X-ray spectroscopy. Saturable absorption is the change of absorbing property of the material which depends on the decrease of the photon absorption cross-section over the course of pulse duration. The decrease of interaction cross section in saturable absorption is due to the depletion of the ground state electrons within the system.

The complexity of SASE pulse structure makes essential the knowledge of nonlinear absorption yields in the experimental data analysis. In this work, the rate-equation model of photon-matter interaction through sequential and simultaneous multiphoton absorption is proposed as a simple, yet effective tool for investigating the influence of SASE pulses' temporal structure on the nonlinear effect yields [5,6]. The SASE pulses' temporal structure may be simulated by use of analytical approximation for both Gaussian and Lorentzian envelopes including the pseudo-random generator. This approach provides good control over the simulated pulses' parameters. The model for interaction is composed of four states: ground, intermediate or virtual states, and final, ionized, state. The interaction model includes both sequential and simultaneous variants of absorption and calculations presented were performed for both, below and above the K-shell ionization threshold energy. Knowing the pulse parameters and their influence on the electronic states' populations will allow for better understanding of the nonlinear phenomena mechanisms and will provide more accurate data analysis procedures. This is of particular importance in the case of nonlinear phenomena na cross-sections measurements.

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PolFEL design.VUV beamline.

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PolFEL is a free-electron laser facility being developed at NCBJ in Poland. The project bases on cooperation of many groups and institutions under consortium agreement (eight polish universities). In addition, close and partly institutionalised collaboration with established and renown operators of FELs in the world offers substantial and invaluable support based on their experience.

The all superconducting electron gun will be in the first phase of the development, a linear superconducting accelerator will be the source of electron beam with the maximal electron energy in the continuous wave (cw) operational regime equal to 160 MeV and 70 MeV for the VUV-line and THz/IR-line, respectively. For the long pulse (lp) operation with a duty factor of 65% the maximal energy of 187 MeV will be available in the VUV-line. Three separate permanent magnets undulators chains will be installed to generate radiation in the spectral regions of THz, IR and VUV. A twosegment superradiant chain will constitute the THz light source, while 11 segments are necessary for VUV SASE chain, and five segments will be needed for IR operating also in the SASE regime. Light pulses will be emitted with the repetition range up to 100 kHz The presented work discusses the photon diagnostic tools for the VUV beamline . The laser-matter interaction group of the Military University of Technology is responsible for the VUV beamline design. The beamline is planned to work alternatively at 70nm (3rd harmonics)and 210 nm (the fundamental wavelength) (nm). The arrangement of the diagnostic tools of the photon beam and the optical elements will be controlled with the light of ~480 nm leaving deliberately tuned undulator. The first monitoring stage of the output photon beam from the undulator will be located directly behind the undulator chain, still in the accelerator concrete tunnel. The distance between the undulator exit and the first beamline optical element (plane mirror) will be about 10 m. This mirror will be located inside a concrete hutch. Along the beamline, the standard diagnostic tools as Cr:YAG scintillators, photodiodes and CCD cameras will be applied in monitoring the position and intensity distribution of the photon beam. However, the absolute photon flux in each shot without visible influence on the photon beam quality will be determined by the gas monitor device (GMD).. The MUT group proposed separation the 3rd harmonics from the fundamental wavelength by applying a customised diffraction grating. Higher diffraction orders of such a device could be applied for the diagnostic aims. It is expected that the beamline will deliver an energy of 100 nJ in a 100 fs pulse at a wavelength of 70 nm while energy of the fundamental component would be equal to 40 μ J in a pulses of the same length. The estimated monochromaticity should be equal to 5-8×10-3. At the moment, the equipment of the user station is under consideration to ensure availability of the pump-probe technique and tunability of the output beam spectrum.

Effect of Auger recombination on transient optical properties in XUV and soft X-ray irradiated silicon nitride

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Spatially encoded measurements of transient optical transmissivity or reflectivity became a standard non-invasive tool for temporal diagnostics of free-electron-laser (FEL) pulses, as well as for the arrival time measurements in X-ray pump - optical probe experiments. The modern experimental techniques can measure optical properties with a temporal resolution below 10 fs. However, carrier transport within the material and out of its surface, as well as carrier recombination may strongly affect the transient optical properties, making the diagnostic measurement inaccurate. Here we report on the detailed analysis performed in 1 how those processes contribute to the transientoptical properties in XUV and soft X-ray irradiated Si3N4 on subpicosecond timescales. Predictions of our model indicate that in both irradiation regimes Auger recombination strongly affects the optical response of Si3N4 after the X-ray triggered ionization process stops. After deconvolving the contributions of Auger recombination and carrier transport, one can regain a high temporal resolution of the FEL pulse properties obtained with a Si3N4 -based diagnostics tool.

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THz diagnostics development for FLASH2020+

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FLASH at DESY has a unique FEL scheme providing soft X-ray beam and intense THz beam simultaneously. The two beams can be used to study matter by pump-probe techniques with only a few femetosecond timing jitter. A project to upgrade FLASH, FLASH2020+, is ongoing at DESY1. After upgrading of the THz beamline, a THz beam with over 250 μ J/pulse and a broader THz bandwith will be transported through the beamline and provided to the users with high repetition rate.

Variable diagnostics tools have been developed at FLASH in order to characterize the THz pulse properties, including power, transverse beam profile, and measurement of the spectrum by Fouriertransform infrared spectroscopy (FTIR). Especially, a THz arrival time tool and a temporal profile characterization have been developed2. It enables the characterization of the THz pulse as a statistical average used in the experiment, with high temporal and spectral resolution.

To efficiently exploit the high THz intensity at FLASH, study an individual transient event in a pumpprobe experiment, and give immediate feedback for THz photon tuning, a single-shot monitor based on electro-optic sampling is under development to determine the THz temporal profile and spectrum at the sample position[3, 4]. The method uses a reflective echelon mirror to generate sequential delays on the spatial positions of the probe laser beam, instead of a mechanic delay stage. It provides 50 fs delay between each probe pulse and covers a 10 ps diagnostic timing window. In addition, an online monitor for THz pulse energy will be installed for FLASH2020+. A spatio-temporal overlap tool for THz-XUV pump-probe experiments is also in development[5].

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Gas Monitor Detectors at Soft X-ray Beamline of PAL-XFEL

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The soft X-ray beamline for X-ray Free Electron Laser (XFEL) of Pohang Accelerator Laboratory (PAL) provides the intense and short soft X-ray pulses in the range 200eV ~ 1200eV. Photon diagnostics devices have been installed at various locations along the beamline. Gas Monitor Detectors (GMD) have been manufactured and installed upstream and downstream of the offset mirrors, thus we can monitor the intensity of photon beam and also observe higher harmonics of photons in the signal shape variation between two GMDs. Two Micro-Channel Plates (MCPs) of the GMD detect electrons and ions created by interaction of XFEL and rare gas and the gas pressure is kept to be under 10⁻⁵ Torr to measure the intensity without affecting the beam. The change of the GMDs signals is checked and compared with different detectors such as photo-diode, different type of MCP and avalanche photo-diode in various test environments. The operation condition of the GMDs are summarized. Results of tests and operation are also presented.

Poster Session

Mechanical Design of Gas Based Detector

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Pohang Accelerator Laboratory X-ray Free Electron Laser (PAL-XFEL) is a research facility, which is designed to generate extremely intense (assuming about 10¹² photons/pulse) and ultra-short (10-200 femtosecond) pulsed X-rays. X-ray Free-Electron Laser (FEL) is characterized by strong pulse-to-pulse fluctuations due to the self-amplified spontaneous emission (SASE) process, and online photon diagnostics has been proven to be indispensable for the experiments. Now, a gas based and inline detector such as gas monitoring detector (GMD) has been developed and tested in PAL-XFEL soft X-ray beamline. Here, the GMD's main engineering points, such as mechanical structure design, simulation, vacuum test process and result are presented.

Pulse-energy damage-thresholds of scintillating screens at the European XFEL diagnostics

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At the European XFEL, diagnostic imagers are placed at several locations along the photon beam transport path towards the experimental stations to deliver information on beam position, shape, pointing, and other beam properties. These imagers use scintillating screens to visualise the x-ray beam. Under certain conditions the x-ray beam intensity may exceed the damage threshold of the scintillators. In this contribution we will describe these conditions, the evaluation of damage thresholds for various materials, and the implementation of an alert system to avoid such damages.

X-ray beam damage to materials may be a result of long term degradation or it may be caused by instantaneous destruction. For imagers at the European XFEL mainly the latter damage is observed by single, short, and intense pulses or sequences of such pulses. The damage threshold is related to the absorbed energy density in the scintillating screens in a given time. This threshold can be evaluated when the transverse XFEL beam intensity distribution is known, which varies along the beam path as a result of focusing and which depends on photon energy and attenuation. Energy dissipation in the screen is not relevant within a pulse of 100 fs or shorter but has an influence on the accumulated energy density of MHz pulse trains.

X-ray Gas Monitor diagnostics at European XFEL operated under special bunch patterns

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One straightforward mode to operate European XFEL is to use all electron bunches passing through the undulator for Self-Amplified Spontaneous Emission (SASE) lasing. In addition, other advanced patterns are available for the users. 1 Fresh-bunch mode: Selectable electron bunches in the train can be dedicated for lasing in SASE1 while being suppressed for lasing in SASE3 and vice versa. The sequence of dedicated and suppressed bunches can be tuned almost freely within some limitations of the machine. 2 Pulse-on-de-mand mode: All bunches are suppressed until the user asks for one or more dedicated pulses in one train. 3 5 Hz mode: The machine still runs at 10 Hz, but one train contains only SASE1 dedicated bunches while the consecutive train has only SASE3 dedicated ones. Even more complicated bunch patterns are realized, where an alternating sequence over many trains can be programmed. All possible pulse delivery situations must be covered by the photon diagnostics, in particular by the permanently and automatically acquiring X-ray Gas Monitors (XGMs). In this contribution we will describe how the diagnostics of these various oper-ation modes are realized and show experimental results.

Io monitor for x-ray free-electron laser pulses in the nJ regime

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X-ray free-electron lasers (FELs), such as the free-electron laser in Hamburg (FLASH), offer optimal conditions for time-resolved studies due to the combination of element specificity of x-rays and short pulses in the fs-range. FELs using super conducting accelerator technology additionally allow very high pulse frequencies and enable the observation of rare events or the investigation of very dilute targets within reasonable time frames.

However, the statistical nature of the photon pulse generating self-amplification spontaneous emission process causes pulse-to-pulse fluctuations in all beam parameters, for example, the pulse energy, wavelength and spectral features. High resolution spectroscopic measurements are sensitive to these fluctuations, which can limit the achievable resolution or might result in data misinterpretation if not considered. To perform high resolution photoelectron spectroscopy a monochromatized beam, which has to be attenuated by up to several orders of magnitude, and the knowledge of the photon numbers per pulse are essential. While the initial pulse energy of the FEL is measured with a gas monitor detector, a monochromator can be used to reduce the FEL bandwidth. The drawback of using a monochromator and cutting out a part of the pulse spectra for the experiment is the loss of the pulse energy information which was measured upstream for the whole pulse. Therefore, pulse energy measurements downstream the monochromator are required to evaluate the number of photons on the sample for every pulse.

Here we present the setup and first results of an IO monitor for the plane grating monochromator beamline of FLASH which is capable to parasitically measure relative shot-to-thot photon pulse energy at the high pulse repetition frequency of 1 MHz. The detector is based on the collection of photoelectrons emitted from a thin film filter. At the cost of a fraction of absorbed photons using solid thin filters as target material has the advantage of a compact design and sensitivity down to the nJ regime enabling pulse energy information for the 3rd harmonic or strongly attenuated beam, which is required for some very pulse intensity sensitive experiments. The variation of filter thickness and material offers a high flexibility and an operating range from 22 nm to 1.5 nm, which is close to the whole wavelength range of FLASH.

Thin Silicon Carbide X-ray Beam Position Monitors for Beam Di- agnostic and Stabilization

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The Swiss Light Source (SLS) generates high brilliance (>1 kW/cm²) coherent and polarized X-ray beam for e.g. diffraction and spectroscopic experiments conducted at the different beamlines. Beam stability is a key issue to increase throughput and resolution, especially in the case of beams with micron sizes or below. This drove the demand for in-line, continuous, accurate and reliable monitoring of the beam position. Semiconductor based X-ray Beam Position Monitors (XBPMs) are front-to- back 4-quadrant detectors which provide continuous spatial and intensity information allowing, e.g. implementation of feedback loops to correct beam instabilities.

In this work, we present experimental results of novel in-line XBPM based on 4H-SiC. The material shows excellent mechanical, thermal and electrical properties. Moreover, the processing of SiC shows a high level maturity due to its industrial applications in power devices. Thanks to its superior characteristics, 2 μ m thin SiC-based XBPMs exhibit a high transmittance (> 0.99 for beam energies larger than 12 keV), energy linearity and larger signal-to-noise ratio compared to polycrystalline-diamond-based XBPMs. Additionally, the implementation of feedback loops, based on SiC – XBPMs, to correct the position of the beam during energy scans at the microXAS beamline at SLS is presented in this work.

Poster Session

Characterization of graphitic wire electrodes within a CVD diamond X-ray pixel detector

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A new type of diamond detector has been developed for use as a transmissive diagnostic instrument for synchrotron X-ray beamlines. The detector utilizes a single-crystal CVD diamond plate as the detector material, with conductive graphitic wires buried within the bulk diamond acting as electrodes. These graphitic electrodes are written in-situ using a pulsed laser-writing technique. The result is that within the instrument's X-ray aperture there is no surface metallisation that could absorb X-rays, or introduce absorption edges that could affect synchrotron experiments. Within the aperture there are no surface structures that could be damaged by exposure to synchrotron radiation beams. A prototype 10x10 pixel detector has previously been fabricated and tested, with all pixels capable of being read out simultaneously using a novel modulation lock-in method. In this paper, laboratory benchtop measurements of the wire conductivity is compared to measurements obtained using X-ray beam induced current (XBIC). Measurements of the electrical properties of the laser-written graphitic wires, and the cross-talk between different wires, are obtained using a spectrum analyser. These results are presented to help determine if there are any fundamental limitations in the lock-in readout technique that has been developed.

Beam Intensity and Position Monitoring at the Hard X-ray PAL- XFEL

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The Pohang Accelerator Laboratory X-ray Free-Electron Laser (PAL-XFEL) is being operated for scientific experiments to provides intense ultrashort X-ray pulses based on the self-amplified spontaneous emission (SASE) process. X-ray Free-Electron Laser (FEL) is characterized by strong pulse-to- pulse fluctuations due to SASE process. Therefore, non-destructive shot-to-shot photon diagnostics has to be implemented to the beamline. The quadrant beam position monitors (QBPMs) that detect backscattered X-rays from a semitransparent thin film placed in the beam path are installed and are being operated at the hard X-ray beamline of the PAL-XFEL. The thin films consist of chemical vapor deposition-acquired diamond and SiNx membranes of various thickness, thus proper film could be chosen depending on photon energy. The QBPMs are calibrated for intensity and position monitoring, and performances are checked through various tests. In here, calibration and performance test results of the QBPM are presented including introduction of the QBPM itself. The intensity and position monitoring results of the hard X-ray FELs are also reported.

Correlation of wavefront modeling and caustic measurements for focusing beamlines at FLASH

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Highly accurate wavefront modeling of the photon-beam is indeed very helpful to predict its behavior at the end of the beamline. At FLASH we used WavePropaGator (WPG), an interface of the SRW code to simulate the caustics of our focusing beamlines. By using WPG, we diagnose our three focusing beamlines at FLASH: BL2, BL3 and FL24. The first two use ellipsoidal mirrors to focus the beam at 2 m. They are installed at the FLASH 1 Hall. FL24 focuses using a bendable Kirk-Patrick Baez optical system and it is installed at the FLASH 2 Hall. During our measurements, we observed important diffraction effects due to the interaction of the radiation and the residual corrugation in the optics. They become more accentuated nearby the focus.

WPG is based on Python scripts and therefore it allows re-define the optical elements or define new components based on the existing ones. All the parameters affecting the source, the transport of the beam or changing the profile distribution need to be included in the simulatio, or at least as much parameters as possible. We observed that including mirror's adjustment, i.e., roll, pitch and yaw along the propagation, increases notably the agreement between the calculated caustic and the measured one, up to 80%.

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Wavefront Sensing and Optics Characterisation at EUV regime with the Fourier Demodulation Technique

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At Free-Electron Lasers (FELs) facilities, wavefront sensing is an essential prerequisite to optical instrument alignments, obtaining knowledge of the focal spot, and collecting feedback for the photon diagnostics. At the Free-electron LASer at Hamburg (FLASH), the Hartmann Wavefront Sensing (HWS) technique has found an established and reliable application to characterize EUV pulses on a single-shot basis and enable further optical aberration analysis. A Hartmann wavefront sensor, in principle, consists of an array of pinholes and a camera downstream in the near field distance. For each pulse, a series of discrete diffraction patterns is measured.

Typically, the centroiding method governs the wavefront retrieval algorithm of the HWS technique. The wavefront slopes are calculated as the displacements between the measured centroids of discrete diffraction patterns and a measured reference centroid set, all within the defined sub-windows.

Defining accurate sub-windows demands a relatively large pitch size, which reduces the wavefront recovery resolution. On the other hand, the sub-windowing approach limits the technique's ability to measure highly distorted wavefronts straying out centroids from the predefined windows.

In this work, we propose applying the Fourier Demodulation (FD) technique as an alternative approach to characterize single-shot EUV wavefronts. The FD technique treats the measured discrete intensity as a whole and calculates the slopes of the wavefront in the Fourier space. The slopes then are integrated with a Hilbert transformation. Thus, the windowing limit is automatically dealt with, and a higher resolution wavefront recovery and high-NA optics characterization are possible. Also, the relaxed constraints enable using this technique in a broader wavelength range that meets the operation wavelengths after the FLASH source upgrade.

We present a theoretical study on the FD technique, as well as a series of forward simulations with varying wavefronts. Preliminarily results of the FD wavefront sensing technique at FLASH2 for the midand high-NA objectives will be discussed.

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