Workshop on SAXS@XFELs and HI & HE laser driven matter

Report of Contributions

Contribution ID: **2** Type: **Talk**

Surface dynamics of warm dense plasmas upon high-intensity laser irradiation investigated by grazing-incidence x-ray surface scattering

Thursday 4 November 2021 14:15 (35 minutes)

Observing ultrafast laser-induced structural changes in nanoscale systems is essential for understanding the dynamics of intense light-matter interactions. For laser intensities on the order of 10^{14}W/cm^2, highly-collisional plasmas are generated at and below the surface. Subsequent transport processes such as heat conduction, electron-ion thermalization, surface ablation and resolidification occur at picosecond and nanosecond time scales. Imaging methods, e.g. using x-ray free-electron lasers (XFEL), were hitherto unable to measure the depth-resolved sub-surface dynamics of laser-solid interactions with appropriate temporal and spatial resolution. Here we demonstrate picosecond grazing-incidence small-angle x-ray scattering (GISAXS) from laser-produced plasmas using XFEL pulses. Using multilayer (ML) samples, both the surface ablation and subsurface density dynamics are measured with nanometer depth resolution. Our experimental data challenges the state-of-the-art modeling of matter under extreme conditions and opens new perspectives for laser material processing and high-energy density science.

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Presenter: RANDOLPH, Lisa (Universität Siegen)

Session Classification: Talks

Contribution ID: **3** Type: **Talk**

SAXS mirror

Friday 5 November 2021 09:50 (25 minutes)

In recent years, a HAPG crystal was designed, tested, and used at HED, XFEL to deflect the SAXS signal from the XFEL beampath, in order to allow shielding of the detector for SAXS signal. In this talk we present the design overview, basic parameters & first results of this instrument.

Primary author: SMID, Michal (HZDR)

Presenter: SMID, Michal (HZDR)

Session Classification: Talks

Contribution ID: **4** Type: **Work in progress**

Reconstruction of SAXS Data using Neural Networks

Thursday 4 November 2021 16:05 (20 minutes)

We aim to simplify the process of reconstructing electron densities from SAXS images by employing a special Neural Network architecture, the conditional Invertible Neural Network (cINN). The only requirement is a simulation from electron density to diffraction image to generate a training dataset. Once trained, it can make accurate and fast (ms range) predictions on simulated and experimental data and furthermore resolve ambiguities resulting from the phase problem. Some challenges remain though, since we cannot differentiate between accurate predictions and false predictions from experimental data not covered by the training dataset (out-of-distribution data) as the output does not convey the degree of certainty of the prediction made by the cINN.

Primary author: THIESSENHUSEN, Erik (HZDR)

Presenter: THIESSENHUSEN, Erik (HZDR)

Session Classification: Talks

Contribution ID: **5** Type: **Talk**

Synthetic probing of ionization dynamics in the solid density plasmas driven by relativistic laser pulses using resonant SAXS

Friday 5 November 2021 13:35 (25 minutes)

Understanding the ionization dynamics is fundamentally important in the interaction of a relativistic laser pulse with a solid density target. In this talk, firstly we present the particle-in-cell (PIC) simulations with various collisional ionization and potential models, showing the target heating, magnetic instabiltiy and plasma resistivity are highly model-dependent \cite{Huang2016,Huang2017}. Secondly, we propose to probe the evolution of ionic density at specific bound-bound resonances by scanning the XFEL photon energy via established SAXS method, which is cable to access the spatial–temporal resolution down to few nanometers and femtoseconds simultaneously. The plasma opacity plays a key role of the XFEL absorption, which in turn affects the resonant SAXS pattern contributed by the imaginary part of ionic scattering form factor\cite{Kluge2016}. We present the calculation of plasma opacity using the atomic collisional-radiative code SCFLY and further simulate the synthetic resonant SAXS imaging pattern which shows strong asymmetric feature. Our recently performed experiment reveals the connection of the temporal evolution of the asymmetry signal and ionization dynamics \cite{Gaus2020}.

[1] L. G. Huang, T. Kluge, and T. E. Cowan, Physics of Plasmas23, 063112 (2016).[2] L. G. Huang, H. P. Schlenvoigt, H. Takabe, and T. E. Cowan, Physics of Plasmas24, 103115 (2017).
[3] T. Kluge, M. Bussmann, H.-K. Chung, C. Gutt, L. G. Huang, M. Zacharias, U. Schramm, and T. E.Cowan, Physics of Plasmas23, 033103 (2016).
[4] L. Gaus, L. Bischoff, M. Bussmann, E. Cunningham, C. B. Curry, E. Galtier, M. Gauthier, A. L.Garc´ıa, M. Garten, S. Glenzer, J. Grenzer, C. Gutt, N. J. Hartley, L. Huang, U. H¨ubner, D. Kraus,H. J. Lee, E. E. McBride, J. Metzkes-Ng, B. Nagler, M. Nakatsutsumi, J. Nikl, M. Ota, A. Pelka,I. Prencipe, L. Randolph, M. R¨odel, Y. Sakawa, H.-P. Schlenvoigt, M.˘Sm´ıd, F. Treffert, K. Voigt,K. Zeil, T. E. Cowan, U. Schramm, and T. Kluge, "Probing ultrafast laser plasma processes insidesolids with resonant small-angle x-ray scattering,"(2020), arXiv:2012.07922 [physics.plasm-ph].

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Presenter: HUANG, Lingen (Helmholtz-Zentrum Dresden-Rossendorf)

Session Classification: Talks

Contribution ID: **7** Type: **Talk**

Targets for SAXS experiments

Friday 5 November 2021 09:25 (25 minutes)

Primary author: PRENCIPE, Irene

Presenter: PRENCIPE, Irene

Session Classification: Talks

Contribution ID: **8** Type: **Talk**

Diamond formation kinetics in shock-compressed C-H-O samples via small angle X-ray scattering and X-ray diffraction

Friday 5 November 2021 10:35 (25 minutes)

Icy giant planets such as Neptune and Uranus are abundant in our galaxy. The interiors of these celestial objects are thought to be mainly composed of a dense fluid mixture of water, methane and ammonia[1]. Due to the high pressure and high temperature conditions deep inside the planet, this material mixture will likely undergo chemical reactions and structural transitions[2]. An example of these reactions is the possible dissociation of hydrocarbons, and subsequent phase separation, allowing the formation of diamonds. Laser shock experiments in combination with an XFEL allowed us to address these questions.[3-5] Due to the presence of water and therefore large amounts of oxygen inside the ice giants, ínvestigating C-H-O samples provides a more realistic scenario than studying pure hydrocarbon systems.

As an ultra-sensitive diagnostic technique, small angle X-ray scattering (SAXS)[6] can explore feature sizes in the order of nanometers by recording their scattering at small angles (typically 0.1-10°), allowing us to obtain deeper insights into the question how diamonds are formed, what grain sizes are achieved and how many grains are formed.

Experiments were carried out at the MEC end station of the LCLS XFEL in December 2020. Three oxygenated polymers with different carbon to H2O ratios, polyethylene terephthalate (PET, C10H8O4), polylactic acid (PLA, C3H4O2) and cellulose acetate (CA, C10H16O8) were compressed to planetary interior states ranging from 50 GPa to 150 GPa and 2000K to 7000K by laser-driven single shocks. The compressed samples were probed utilizing in situ X-ray diffraction (XRD) and SAXS. The diamond formation kinetics in presence of oxygen in these three materials have been observed. SAXS shows more sensitive information than XRD, revealing that the diamond fraction first increases and then decreases with increasing of pressure and the growth of particles with time in the medium pressure regime (~110 GPa). The observed particle radius of diamond is between 1.5 nm and 3 nm. In addition, the proportion of carbon in the initial sample materials also shows a correlation with the observed diamond fraction. Ongoing simulations aim to explain these phenomena in order to improve the theory of planetary formation and evolution.

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[2]M. Ross, Nature 292, (1981).
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[4]D. Kraus, N. Hartley, S. Frydrych, et al., Phys. Plasmas 25, (2018).
[5]A. Schuster, N. Hartley, J. Vorberger, et al., Phys. Rev. B 101, (2020).
[6]O. Glatter, O. Kratky and H. Kratky, Small angle X-ray scattering (Academic press, 1982).

Primary authors: HE, Zhiyu (Helmholtz-Zentrum Dresden-Rossendorf); Mr LUTGERT, Julian (Helmholtz-Zentrum Dresden-Rossendorf); Dr VORBERGER, Jan (Helmholtz-Zentrum Dresden-Rossendorf, Dresden); Prof. KRAUS, Dominik (Universität Rostock, Rostock, Germany)

Presenter: HE, Zhiyu (Helmholtz-Zentrum Dresden-Rossendorf)

Session Classification: Talks

Contribution ID: **9** Type: **Work in progress**

Machine Learning in GISAXS reconstruction

Thursday 4 November 2021 15:45 (20 minutes)

Primary author: LIU, Yichao

Co-authors: Dr RANDOLPH, Lisa (Siegen University); Dr KLUGE, Thomas (HZDR); Dr HOFFMANN, Nico (HZDR); Dr GANEVA, Marina (Jülich center)

Presenter: LIU, Yichao

Session Classification: Talks

Contribution ID: **10** Type: **Talk**

X-ray radiation transport in GPU accelerated Particle In Cell simulations

Friday 5 November 2021 15:50 (20 minutes)

Ultra-high-intensity laser pulse interactions with solid density targets are of central importance for modern accelerator physics, Inertial Confinement Fusion(ICF) and astrophysics.

In order to meet the requirements of real-world applications, a deeper understanding of the underlying plasma dynamics, including plasma instabilities and acceleration mechanisms, is needed.

Due to high electron density, the over-dense target bulk is impenetrable to probes in the optical range.
Hence, several X-ray diagnostics, such as small-angle X-ray scattering (SAXS) and X-ray polarimetry, were proposed by the community.

Therefore, we bring a Monte Carlo based X-ray radiation transport module into our Particle In Cell simulation framework PIConGPU. Among others, this allows for Thompson scattering, e.g. for SAXS, and Faraday effect calculation for polarimetry - as online, in-situ diagnostics.

Primary author: ORDYNA, Pawel

Co-authors: KLUGE, Thomas (HZDR); SCHRAMM, Ulrich; COWAN, Thomas E. (HZDR)

Presenter: ORDYNA, Pawel

Session Classification: Talks

Contribution ID: **11** Type: **Talk**

Using GISAXS to observe Density Oscillation in Multi Layer Targets

Thursday 4 November 2021 14:50 (20 minutes)

Presenting results of simulations showing the density oscillation. The density oscillation describes the oscillation of the single layers in width and density in a multi layer target. We will see how the the GISAXS method allows to observe this dynmamic.

Primary author: PASCHKE-BRUEHL, Franziska-Luise

Presenter: PASCHKE-BRUEHL, Franziska-Luise

Session Classification: Talks

Contribution ID: **12** Type: **Talk**

Probing ultrafast plasma expansion using SAXS

Primary author: KLUGE, Thomas (HZDR)

Presenter: KLUGE, Thomas (HZDR)

Session Classification: Talks

Contribution ID: **13** Type: **Talk**

Probing laser-solid interactions with Resonant Small-Angle X-ray Scattering

Friday 5 November 2021 15:30 (20 minutes)

SAXS has been applied in two beam times at LCLS (2014, 2018) in order to study the plasma expansion dynamics following the interaction of solid-density samples with an ultrahigh intensity laser. The first experiment demonstrated, that SAXS in combination with nanostructured grating targets enables to measure the plasma surface expansion with fs and nm resolution [Kluge et al., Phys. Rev. X 8, 031068 (2018)]. In the follow-up experiment, the pump laser intensity reached the relativistic intensity regime and allowed for the generation of highly ionized plasma states. In this scenario, probing at resonant X-ray energies has shown to give new insight into the ionization process, plasma opacity and density dynamics by studying asymmetries in SAXS patterns [Gaus et al., arXiv: 2012.07922 (under review)]. This talk aims to give an overview on the experimental results from these experiments with respect to resonant SAXS.

Primary authors: GAUS, Lennart (HZDR); Dr BISCHOFF, L; Dr BUSSMANN, M; Mr CUNNINGHAM, E; Mr CURRY, C. B.; Mr E, J; Mr GALTIER, E; Mr GAUTHIER, M; Mr GARCIA, A. L.; Mr GARTEN, M; Prof. GLENZER, Siegfried; GRENZER, J; Prof. GUTT, C.; Mr HARTLEY, N. J.; HUANG, L; HÜBNER, U.; Prof. KRAUS, D; LEE, H. J.; MCBRIDE, E. E.; METZKES-NG, J; NAGLER, B; NAKATSUTSUMI, M; NIKL, J; OTA, M; PELKA, A; PRENCIPE, I; RANDOLPH, L; RÖDEL, M; SAKAWA, Y; SCHLENVOIGT, H.-P.; SMID, M; TREFFERT, F; VOIGT, K; ZEIL, K; Prof. COWAN, T. E.; Prof. SCHRAMM, U.; KLUGE, T

Presenter: GAUS, Lennart (HZDR)

Session Classification: Talks

Contribution ID: **14** Type: **Talk**

Targetry for revealing laser-driven nanostructures in SAXS and GISAXS experiments with high repetition rate

Friday 5 November 2021 09:00 (25 minutes)

The first experiments with ultrafast SAXS and GISAXS using free-electron lasers have shown effects such as plasma expansion from micro- or nanostructured targets, for example clusters, gratings, wires or multilayers. These targets produce pronounced features in the SAXS and GISAXS signal due to their geometry. For investigating plasma instabilities or surface plasma waves, which have very subtle SAXS signatures, targetry with smooth planar geometry would be advantageous. High repetition rate targetry, for example liquid leaf targets and tape targets are discussed, which can facilitate parametric scans in SAXS and GISAXS experiments.

Primary author: RÖDEL, Christian (TU Darmstadt)

Presenter: RÖDEL, Christian (TU Darmstadt)

Session Classification: Talks

Contribution ID: **15** Type: **Talk**

Combined single-shot Small Angle X-Ray Scattering and Phase Contrast Imaging in ultra-intense laser-matter interactions at euXFEL

Friday 5 November 2021 14:00 (25 minutes)

The High Energy Density (HED) instrument at the European XFEL provides a platform to study hot and warm dense matter. The Helmholtz International Beamline for Extreme Fields (HiBEF) is the User Consortium supplying HED with two laser systems (the high-intensity ReLaX laser, by Amplitude Technologies, and the high-energy Dipole-100X laser, by STFC), Diamond Anvil Cells setup and high-pulsed magnetic fields. These tools in combination with the XFEL beam enable the investigation of relativistic laser plasmas, strong-field QED phenomena, high-pressure astro- and planetary physics as well as magnetic phenomena in condensed matter.
The commissioning of the ultra-short pulse high-intensity relativistic laser at XFEL, ReLaX, provides new unique opportunities in the plasma and high-field physics fields. ReLaX is a double CPA Ti:Sa laser delivering 100 TW pulses on target, reaching intensities up to 10^{20} W/cm^2.
Small-Angle X-Ray Scattering (SAXS) without the need of a beamstop was first commissioned at HED in September 2019. Two high-annealed pyrolytic graphite (HAPG) crystals were used to reflect the SAXS photons onto a detector while allowing the main XFEL beam to go through. In April and May 2021, Small-Angle X-Ray Scattering (SAXS) and Phase Contrast Imaging (PCI) were simultaneously demonstrated in pump-probe experiments at HED.
In this talk, we discuss the challenges on combining these X-Ray techniques in the harsh environment generated by the laser-matter interaction. We will also show results on the combined SAX and PCI measurements of hole boring in wire targets.

Primary authors: LASO GARCIA, Alejandro (HZDR); TONCIAN, Toma (HZDR); HOEPPNER, Hauke (HZDR); PELKA, Alexander (HZDR); BAEHTZ, Carsten (HZDR); BRAMBRINK, Erik (European XFEL); NAKATSUTSUMI, Motoaki (European XFEL); SCHWINKENDORF, Jan-Patrick (European XFEL); PRESTON, Thomas (European XFEL); COWAN, Thomas (HZDR); ZASTRAU, Ulf (European XFEL); SCHLENVOIGT, Hans-Peter (HZDR); PRENCIPE, Irene (HZDR); KONOPKOVA, Zuzana (European XFEL)

Presenter: LASO GARCIA, Alejandro (HZDR)

Session Classification: Talks

Contribution ID: **16** Type: **Talk**

Considerations for single-pulse phase contrast imaging at HED

Friday 5 November 2021 14:25 (25 minutes)

Primary author: HAGEMANN, Johannes

Presenter: HAGEMANN, Johannes

Session Classification: Talks

Contribution ID: **18** Type: **Tutorial**

Asymmetries in resonant SAXS

Friday 5 November 2021 15:10 (20 minutes)

Primary author: KLUGE, Thomas (HZDR)

Presenter: KLUGE, Thomas (HZDR)

Session Classification: Talks

Contribution ID: **19** Type: **Talk**

openPMD - A Scientific, Community Meta-Data Standard

Thursday 4 November 2021 16:40 (25 minutes)

The open standard for particle-mesh data (openPMD) is a FAIR community standard. openPMD meta-data adds scientific self-description in a machine-actionable format to data sets, which allows sharing data processing frameworks, chaining data through simulations and designing long analysis pipelines. Developed in the open as a FAIR data standard, openPMD is based on portable and scalable file formats such as HDF5 and ADIOS2, among others. In this talk, we will present the community principles, existing implementations, recent research results for file and file-less analysis, and possible integration directions.

Presenter: HÜBL, Axel (LBNL)

Session Classification: Talks

Contribution ID: **20** Type: **Talk**

Benchmarking autonomous scattering experiments illustrated on TAS

Friday 5 November 2021 11:50 (25 minutes)

With the advancement of artificial intelligence and machine learning methods, autonomous approaches are recognized to have great potential for performing more efficient TAS experiments. In our view, it is crucial for such approaches to provide thorough evidence about respective performance improvements in order to increase acceptance within a community. Therefore, we propose a benchmarking procedure designed as a cost-benefit analysis that is applicable not only to TAS, but also to any scattering method sequentially collecting data during an experiment. For a given approach, the performance assessment is based on how much benefit, given a certain cost budget, it is able to acquire in predefined test cases. Different approaches thus get a chance for comparison and can make their advantages explicit and visible. In the talk, we specify the key components of the benchmarking procedure for a TAS setting and try to motivate ideas for an audience with a more general background in scattering.

Presenter: PARENTE

Session Classification: Talks

Contribution ID: **21** Type: **not specified**

Potential benefits of electronic damage in x-ray imaging

Friday 5 November 2021 11:25 (25 minutes)

Ionization is generally considered detrimental to the quality of single exposure images recorded with ultra bright
modern X-ray sources, such as X-ray free electron lasers (XFELs). We conducted a X-ray coherent diffraction
imaging (CDI) study at the Linac Coherent Light Source (LCLS) on single rare gas nanoparticles. Our results indicate
that the X-ray scattering cross section may increase due to transient ionic resonances before structural damage
degrades the image. We also observe that the samples become increasingly transparent if the pulse parameters
correspond to typical values of single particle imaging experiments. Dynamical electronic structure calculations
attribute the observed effects to electronic damage and predict amplification of X-ray coherent scattering of up to two
orders of magnitude compared to the neutral scattering cross section might be possible. We also demonstrate that
ionic resonances are present in images recorded with sub-fs pulses which proves that transient resonances can be
exploited before ionic damage.

Presenter: KUSCHEL, Stephan (DESY)

Session Classification: Talks

Contribution ID: **22** Type: **Talk**

openPMD

Friday 5 November 2021 16:10 (20 minutes)

The openPMD-api is a library for the description of scientific data according to the Open Standard for Particle-Mesh Data (openPMD). Its approach towards recent challenges posed by hardware and workflow heterogeneity lies in the decoupling of data description in domain sciences from concrete implementations in hardware and IO. This is reflected in the openPMD standard which defines the logical structure, but not the physical implementation of scientific data. This seminar talk gives an introduction on the openPMD standard as well as the openPMD-api. Two live demonstrations show how to write and read openPMD data in Python, and how to visualize openPMD data in the openPMD-viewer.

Presenter: PÖSCHEL, Franz (CASUS)

Session Classification: Talks

Contribution ID: **23** Type: **Talk**

Overview to ML-based reconstruction techniques

Thursday 4 November 2021 15:25 (20 minutes)

We will be learning about most recent machine learning techniques for solving ill-posed inverse problems such as SAXS reconstruction.

Primary author: HOFFMANN, Nico (HZDR)

Presenter: HOFFMANN, Nico (HZDR)

Session Classification: Talks

Contribution ID: **24** Type: **Talk**

SAXS measurement of sub-micron solid-density columnar plasma expansion induced by a high-intensity laser at SACLA

Friday 5 November 2021 11:00 (25 minutes)

Application of small-angle x-ray scattering (SAXS) to a measurement of the temporal evolution of plasma expansion with nanometer spatial and femtosecond temporal resolution was established recently [1]. Here a grating target with a sub-micron structure was irradiated by a high-intensity laser pulse, and the grating expansion in the lateral direction was probed by an XFEL pulse. In our research, we utilized a silicon rod assembly with a sub-micron structure as a target instead of a grating, that is the dimension of the structure is extended from two to three. The temporal evolution of the columnar plasma induced by a high-intensity laser pulse was probed by SAXS changing the diameter and interval of the rods. In this talk, the advantages and disadvantages of SAXS for the three-dimensional structure will be discussed.
[1] Kluge et al., Phys. Rev. X 8, 031068 (2018).

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Presenter: OTA, Masato

Session Classification: Talks

Contribution ID: **25** Type: **Talk**

Ionic liquids with/without small water content confined in porous glasses

Friday 5 November 2021 13:10 (25 minutes)

The structure and dynamics of the ionic liquid 1-ethyl-3-methylimidazolium acetate (EMIMAc) in porous glass with pores of the size 40 and 100 Å is determined in comparison to the bulk liquid [1]. We employed x-ray diffraction to measure the domain structure, and neutron backscattering for the dynamics. In confinement, the liquid displays onion-like domain structuring while in bulk the liquid is largely forming a bicontinuous structure similar to microemulsions. This also has an effect on the dynamics of the liquid at high temperatures (373K): The ions in the bulk can diffuse along the domain boundaries while they need to cross the domains in the ordered state in confinement. At low temperatures, the attractive forces of all ions are such strong –we have a highly viscous fluid –such that the diffusion in any direction is similarly slow, and the exact domain structure does not affect the diffusion mechanism. The addition of ½ mol/mol water slightly increases the correlation length and accelerates the dynamics while the water and acetate seem to be rather tightly bound to each other.

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Presenter: FRIELINGHAUS, Henrich (Forschungszentrum Jülich GmbH)

Session Classification: Talks

Contribution ID: **26** Type: **not specified**

Laser driven magnetic filaments in relativistically transparent plasmas as a platform for high-field science

Thursday 4 November 2021 17:05 (25 minutes)

High-power high-intensity multi-beam laser systems that are becoming operational around the world can now be used to create a platform for high-field science that is based on relativistically transparent magnetic filaments driven by irradiating lasers within a dense plasma. The strength of the quasistatic field can be comparable to that of the laser, reaching the multi-GG level. This talk will review several phenomena that can be studied with experimentally achievable laser intensities at multi-PW laser facilities. These include emission of dense gamma-ray beams in the quantum regime and electron-positron pair creation from light alone. Astrophysical environments are known for exotic physics regimes that involve generation of extreme magnetic fields and creation of matter and antimatter from light alone. The discussed platform provides a potential path towards recreating relevant regimes in laboratory conditions.

Presenter: AREFIEV, Alexey (UC San Diego)

Session Classification: Talks