The 4th PAL-XFEL Users' Meeting

July 3-4, 2024

Pohang Accelerator Laboratory

https://pal.postech.ac.kr/2024palxfelum

Invited Speakers

Kyeong Kyu Kim (President of KOSUA, Sungkyunkwan University)
Changyong Song (POSTECH)
David Reis (Stanford University)
Jongwoo Lim (Seoul National University)
Kohei Yamagami (JASRI)
Kwang Yeon Hwang (Korea University)
Kyung Hwan Kim (POSTECH)

PAL POHANG ACCELERATOR LABORATORY

KOSUA 한국방사광이용자협회 The Korean Synchrotron Radiation User's Association

Ministry of Science and ICT

The 4th PAL-XFEL Users' Meeting

PAL-XFEL

JULY 3~4, 2024

주최 : 포항가속기연구소

주관 : (사)한국방사광이용자협회

후원 : 과학기술정보통신부

The 4th PAL-XFEL Users' Meeting

July 3 (Wed)					
12:00~13:00	Registration				
13:00~13:10	Welcome Remarks				Dr. Heung-Sik Kang PAL
13:10~13:40	Status Reports				Dr. Intae Eom PAL
13:40~14:10	Invited Talk I Nucleic Acids Research: From Basic Science to Clinical Applications				Prof. Kyeong Kyu Kim Sungkyunkwan Univ.
14:10~14:30	Coffee break				
14:30~15:00	Invited Talk II Ultrafast Soft X-ray Absorption Study for Valence Transition in Correlated 4f Inter-metallic Compounds On-line				Dr. Kohei Yamagami JASRI
15:00~15:30	Invited Talk III Dynamic strain evolution and lithium distribution in battery particles				Prof. Jongwoo Lim Seoul National Univ.
15:30~16:00	Invited Talk IV Direct femtosecond imaging of materials phase transitions driven far from equilibrium				Prof. Changyong Song POSTECH
16:00~16:30	Group photo & Coffee break				
16:30~18:00	Parallel session				
	Ultrafast Photo-induced Dynamics in Condensed Matter at PAL-XFEL	Exploring Chemical Reaction Dynamics with PAL-XFEL : A Symposium for Young Scientists	Basic Description and Discussion for Successful SFX Experiment	Femtosecond Time Resolved Imaging Experiment	
	Convener Dr. Hoyoung Jang Dr. Sae Hwan Chun	Convener Dr. Jae Hyuk Lee Dr. Sang Han Park	Convener Dr. Sang Jae Lee	Convener Dr. Sunam Kim Dr. Sangsoo Kim Dr. Daewoong Nam	
18:00~20:00	Banquet				
July 4 (Thur)					
09:30~10:00	Invited Talk V Atomic-scale Imaging of Valence Electron Motion in Solids				Prof. David Reis Stanford Univ.
10:00~10:30	Invited Talk VI Advantage of Enzyme Structure Complexed with Cofactor using SFX:3-Hydroxybutyryl-CoA Dehydrogenase from *F. prausnitzii A2-165*				Prof. Kwang Yeon Hwang Korea Univ.
10:30~10:50	Coffee break				
10:50~11:20	Invited Talk VII Experimental Studies of Water's Second Critical Point at PAL-XFEL				Prof. Kyung Hwan Kim POSTECH
11:20~11:35	Poster: One Minute Pitch				
11:35~13:00	Poster Presentation				
13:00~13:30	Poster Awards & Closing				Dr. Intae Eom PAL

The 4th PAL-XFEL Users' Meeting presentation list

No.	No.	Speaker	Affiliation	Abstract
1	IL-01	Kyeong Kyu Kim	Sungkyunkwan Univ.	Nucleic Acids Research: From Basic Science to Clinical Applications
2	IL-02	Kohei Yamagami	JASRI	Ultrafast Soft X-ray Absorption Study for Valence Transition in Correlated 4f Inter-metallic Compounds
3	IL-03	Jongwoo Lim	Seoul National Univ.	Dynamic strain evolution and lithium distribution in battery particles
4	IL-04	Changyong Song	POSTECH	Direct femtosecond imaging of materials phase transitions driven far from equilibrium
5	IL-05	David Reis	Stanford Univ.	Atomic-scale Imaging of Valence Electron Motion in Solids
6	IL-06	Kwang Yeon Hwang	Korea Univ.	Advantage of Enzyme Structure Complexed with Cofactor using SFX: 3-Hydroxybutyryl-CoA Dehydrogenase from *F. prausnitzii A2-165*
7	IL-07	Kyung Hwan Kim	POSTECH	Experimental Studies of Water's Second Critical Point at PAL-XFEL
8	PS-01	Hoyoung Jang, Sae Hwan Chun	PAL	Ultrafast Photo-induced Dynamics in Condensed Matter at PAL-XFEL
9	PS-02	Jae Hyuk Lee, Sang Han Park	PAL	Exploring Chemical Reaction Dynamics with PAL-XFEL : A Symposium for Young Scientists
10	PS-03	Sang Jae Lee	PAL	Basic Description and Discussion for Successful SFX Experiment
11	PS-04	Sangsoo Kim, Sunam Kim, Daewoong Nam	PAL	Femtosecond Time Resolved Imaging Experiment
12	PP-01	Jain Gu (Hyotcherl Ihee)	IBS/KAIST	Ultrafast structural dynamics of I_2 in methanol visualized with femtosecond X-ray liquidography
13	PP-02	Minjeong Ki (Kyung Hwan Kim)	POSTECH	Understanding the Processes Occurring During an 800 nm Optical Laser Probe on Liquid Water
14	PP-03	Haneol Oh (Tae Kyu Kim)	KAIST	Elucidating the effects of sulfur atoms on the photo-induced dynamics of thiouracils using time-resolved X-ray absorption spectroscopy
15	PP-04	JUNU BAE (Tae Wu Kim)	Mokpo National Univ.	Photo-induced spin cross-over dynamics in cytochrome c
16	PP-05	Seonggon Lee (Hyotcherl Ihee)	IBS/KAIST	Application of Single Object Scattering Simulation to Unveil the Fluctuating Structures of Biological Macromolecules
17	PP-06	Jinkyu Lim	Catholic Univ.	Development of hard X-ray spectrometer using Polycapillary optics for XAS measurements of dilute samples at PAL-XFEL
18	PP-07	Tae Gyun Woo (Tae Kyu Kim)	KAIST	Unveiling excited-state molecular dynamics of $Co(AcAc)_3$ using the combined probes of femtosecond X-ray and optical absorption spectroscopy; structural insight for hidden charge-transferred state
19	PP-08	Yunbeom Lee (Hyotcherl Ihee)	IBS	Visualizing the Structural Change of a Metal–Organic Framework Using Femtosecond Serial Crystallography
20	PP-09	Kichan Park (Kyung Hwan Kim)	POSTECH	Elucidating the Melting Dynamics of Crystalline Ice on a Picosecond Timescale Using Time-resolved X-ray Scattering
21	PP-10	Junho Lee ((Tae Kyu Kim)	KAIST	Investigation of Ligand Charge Delocalization Mediated Charge Transfer on the bridged bimetalic complex

The 4th PAL-XFEL Users' Meeting presentation list

No.	No.	Speaker	Affiliation	Abstract
22	PP-11	JiYun Choi (Jun Hyuk Moon)	Korea Univ.	Efficient Conversion of Methane to Ethanol with Fe Single Atom Catalysts
23	PP-12	Minseop LEE (Seung-Min Paek)	Kyungpook National Univ.	X-ray Absorption Spectroscopic Analysis and Phase Engineering of Lepidocrocite-Type Titanate/NiCo-LDH Heterostructured Electrodes
24	PP-13	JungChan Choi (Changyong Song)	POSTECH	Role of Cations to Charge Density Wave in Kagome Metal via Time-resolved X-ray Diffraction
25	PP-14	Jihyeon Hwang (Kyungwan Kim)	Chungbuk National Univ.	Ultrafast lattice dynamics of $SrRuO_3$ and $SrRuO_3/SrTiO_3$ superlattices
26	PP-15	SEOHYOUNG CHANG	Chung-Ang Univ.	Time-resolved RIXS and quantum materials
27	PP-16	Sinwoo Kim (Changyong Song)	POSTECH	Photo induced ultrafast phase-transition of metallic glass directly observed by single-pulse imaging with XFEL
28	PP-17	Sung Soo Ha (Hyunjung Kim)	Sogang Univ.	Time-resolved Ultrafast Strain Evolution in $SrTiO_3$ Nanocrystals by Bragg Coherent X-ray Diffraction Imaging
29	PP-18	Sung Soo Ha (Hyunjung Kim)	Sogang Univ.	Ultrafast DFXM for Light-Induced Structural Evolution
30	PP-19	Junha Hwang (Changyong Song)	POSTECH	Void Nucleation in Ultrafast Photoinduced Melting Revealed by Time-Resolved Coherent Diffraction Imaging
31	PP-20	Jinback Kang	PAL	XFEL beam profile examination for tr-BCDI experiment
32	PP-21	Seungcheol Lee	PAL	Simulation, fabrication, and performance test of Low Gain Avalanche Detector for X-ray detection
33	PP-22	Tae-Kyu Choi	PAL	Time-resolved Hard X-ray Emission Spectroscopies using Self-seeded Pulses at PAL-XFEL
34	PP-23	Daewoong Nam	PAL	Current status of the CXI endstation for revealing structural information at nanoscale resolution
35	PP-24	Sae Hwan Chun	PAL	Hard X-ray FXS instrument for the study of energy and quantum materials
36	PP-25	Sunam Kim	PAL	Introduction to tr-BCDI system at XSS beamline
37	PP-26	Dogeun Jang	PAL	Laser systems for time-resolved experiments at Pohang Accelerator Laboratory X-ray Free-Electron Laser
38	PP-27	Hoyoung Jang	PAL	Resonant Soft X-ray Scattering (RSXS) Endstation at PAL-XFEL
39	PP-28	Jaehyun Park	PAL	A fascinating research platform for biology: Serial femtosecond crystallography endstation
40	PP-29	Sang Han Park	PAL	Latest developments in at XAS/XES endstation
41	PP-30	Jae Hyuk Lee	PAL	Studying of the Chemical Reaction Dynamics at Femtosecond X-ray Liquidography (FXL) Endstation

Abstract of Invited Lecture

[IL-01]

Nucleic Acids Research: From Basic Science to Clinical Applications

K. K. Kim

Department of Precision Medicine, Sungkyunkwan University School of Medicine, Suwon, Korea

Nucleic acids have been major research topics due to their relevance to genetic events in cells. There have been three significant breakthroughs in the field of nucleic acids research. First, in 1953, Watson and Crick proposed the double-helix model of DNA, later supported by many high-resolution structural studies of DNA. Various structural and molecular biology studies on RNA followed, revealing its diverse structure and functions. It was also discovered that DNA can adopt various non-double-stranded forms, expanding the understanding of its regulatory role in genetic events. The second major breakthrough was the achievement of whole genome sequencing, made possible by advancements in sequencing technology and data science. This revolutionized the understanding of molecular biology and molecular medicine, and further opened many new scientific fields such as genome biology and prevision medicine. The third breakthrough, currently unfolding, is nucleic acid therapy. This field involves targeting nucleic acids or genomes and using them or their derivatives as therapeutics. The successful introduction of mRNA vaccines for COVID-19 triggered remarkable progress in this field. Numerous mRNA therapeutics are currently in clinical trials, promising to revolutionize therapeutic options for doctors and patients. In this presentation, I will briefly introduce the history of nucleic acids research and how XFEL technology is contributing to its scientific expansion.

[IL-02]

Ultrafast Soft X-ray Absorption Study for Valence Transition in Correlated 4f Inter-metallic Compounds

Kohei Yamagami, [1]Hiroki Ueda, [2]Urs Staub, [3]Yujun Zhang, [4]Kohei Yamamoto, [5]Sang Han Park, [6]Soonnam Kwon, [6]Akihiro Mitsuda, [7]Hirofumi Wada, [7]Takayuki Uozumi, [8]Kojiro Mimura, [8]and Hiroki Wadati[9]

[1]Japan Synchrotron Radiation Research Institute (JASRI), [2]SwissFEL, [3]Swiss Light Source (SLS), [4]Institute of High Energy Physics (IHEP), [5]National Institutes for Quantum Science and Technology (QST), [6]PAL-XFEL, [7]Dep. of Phys., Kyushu Univ., [8]Dep. of Phys. and Electr., Osaka Metro. Univ, 9Dep. of Mater. Sci., University of Hyogo

Valence transitions in strongly correlated electron systems are caused by orbital hybridization and Coulomb interactions between localized and delocalized electrons. Launching the transition by photoelectric fields can directly excite the electronic states and thus provides an ideal platform to study the correlation among electrons on ultrafast timescales. In this study, we probe the 4f electron states of EuNi2(Si0.21Ge0.79)2 at the sub-ps timescale after photoexcitation by x-ray absorption spectroscopy across the Eu M5-absorption edge. The observed spectral changes due to the excitation indicate a population change of total angular momentum multiplet states J = 0, 1, 2, and 3 of Eu3+ and the Eu2+ J = 7/2 multiplet state caused by an increase in 4f electron temperature that results in a 4f localization process. In addition, this electronic temperature increases combined with fluence-dependent screening accounts for the strongly nonlinear effective valence change. Our results elucidate the energetics of charge fluctuations in valence-mixed electronic systems, which provide enriched knowledge regarding the role of valence transitions and orbital hybridization for quantum critical phenomena.

Ref: K. Yamagami, et al., Phys. Rev. Research 6, 023099 (2024).

[IL-03]

Dynamic strain evolution and lithium distribution in battery particles

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High-Ni layered oxides undergo significant chemomechanical changes when charged above 4.2 V, resulting in crystallographic defects and lattice distortions in the cathode particles. These imperfections are often concealed during discharge, complicating their detection and characterization. Their impact on the structural stability and electrochemical performance of cathode materials remains unclear. This study employs synchrotron-based X-ray diffraction and Bragg coherent diffraction imaging (CDI) to detect subtle yet persistent lattice distortions in the discharged state after high-voltage cycling. In situ Bragg CDI reveals internal strain evolution within the particles upon mild heating, linked to hidden lattice imperfections and structural instability. Particles cycled above 4.2 V show significant strain evolution and domain deformation upon heating, whereas particles cycled below 4.2 V release internal strain and maintain their shape. These findings suggest that hidden lattice imperfections from high-voltage cycling can cause microstructural degradation at high temperatures, undermining the structural stability of high-Ni layered oxide particles and increasing the risk of degradation.

[IL-04]

Direct femtosecond imaging of materials phase transitions driven far from equilibrium

Changyong Song,[1,2,]*Eunyoung Park,[1,2] Sinwoo Kim,[1,2] Junha Hwang,[1,2], Jaeyong Shin,[1,2] Sangsoo Kim[3], Daewoong Nam[3]

1- Department of Physics and Photon Science Center, POSTECH, Pohang 37673, Korea
2- Center for Ultrafast Science on Quantum Matter, Max Planck POSTECH Korea Research Initiative, Pohang 37673, Korea
3- Pohang Accelerator Laborator, Pohang 37673, Korea

Intense femtosecond-laser pulses drive material phase transitions via kinetic reactions otherwise hidden in equilibrium measurements, which stimulates a strong interest in revealing the reaction dynamics of individual atoms prompted by photo-depleted bonding electrons. However, the field of ultrafast atomic dynamics has been limited by the challenges involved in resolving the accompanying irreversible processes at the relevant space−time resolution. By establishing single-pulse time-resolved experimental technique using an X-ray free-electron laser, we overcome this to directly observe the kinetic processes accompanied during the nonequilibrium phase transitions. In this talk, we will introduce recent experimental observations of exotic melting reaction forbidden in thermodynamic (near) equilibrium condition together with physical interpretation guided by the two-temperature molecular dynamics.

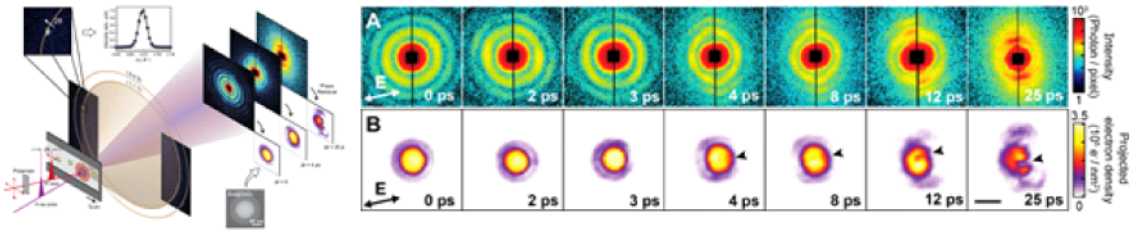

Figure 1. XFEL single pulse time-resolved imaging and diffraction experiments (left). Femtosecond photoinduced melting of the Au@SiO2 single nanoparticles observed by single XFEL pulses (Right). Top panel displays XFEL diffraction patterns and bottom panel display specimen images as projected electron densities on ultrafast melting [1].

References

[1] Jaeyong Shin, Chulho Jung, Yungok Ihm, Seung-Phil Heo, Daewoong Nam, Sangsoo Kim, Minseok Kim, Intae Eom, Ji Hoon Shim, Do Young Noh, and Changyong Song*, "Ultrafast energy transfer process in confined Au nanospheres revealed by femtosecond X-ray imaging and diffraction", Nano Letters 23:1481 (2023).

[2] C. Jung, Y. Ihm, D.-H. Cho, H. Lee, D. Nam, S.-S. Kim, I.-T. Eom, J. Park, C. Kim, Y. Kim, J. Fan, N. Ji, J. R. Morris, S. Owada, K. Tono, J-H Shim, H. Jiang, M. Yabashi, T. Ishikawa, D.-Y. Noh, and C. Song*, "Inducing thermodynamically blocked atomic ordering via strongly driven nonequilibrium kinetics", Science Advances 7:eabj8552 (2021)

[3] Y. Ihm, D. Cho, D. Sung, D. Nam, T. Sato, C. Jung, S-S. Kim, J. Park, S-N. Kim, M. Gallagher-Jones, Y. Kim, R. Xu, S. Owada, J. H. Shim, K.Tono, M. Yabashi, T. Ishikawa, J. Miao, D.-Y. Noh, and Changyong Song*, "Direct observation of picosecond melting and disintegration of metallic nanoparticles", Nature Communications 10:2411 (2019).

[IL-05]

Atomic-scale Imaging of Valence Electron Motion in Solids

D.A. Reis

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X-ray free-electron lasers have emerged as powerful probes of the structure and dynamics of matter on the relevant length and time scales of atomic motion in chemistry and materials. Yet much of chemistry and the functional properties of materials depend on the valence electron density that is only a small fraction of the electron density. Here we will describe recent results on x-ray scattering from optically-driven crystals, where phase-matched nonlinear sum frequency generation is particularly sensitive to the valence electron motion within a unit cell. In this case the scattered x rays appear as sidebands in energy and momentum about the ordinary elastically scattered Bragg peaks and their amplitude is proportional to the magnitude square of the spatial and temporal Fourier components of the driven charge density [1-4]. We present measurements of the first and second order sidebands in single crystal silicon excited below the band gap [5]. We find that the polarization dependence of the second order sideband from a single Bragg peak already reveals important information about the local symmetry of the interstitial electrons, even without knowing the phase of the nonlinear structure factors. Extension of this method to imperfect crystals will allow us to probe the microscopic origins of the strong-field and far-from equilibrium response in a variety of materials. We will thus also describe the first x-ray an optical mixing measurements on MgO using a purpose-built monochromator and analyzer on the PAL-XFEL[5].

[1] P. M. Eisenberger and S. L. McCall. Phys. Rev. A, 3, 1145, 1971.

[2] I. Freund and B. F. Levine. Phys. Rev. Lett., 25, 1241, 1970.

[3] T. E. Glover, D. M. Fritz, M. Cammarata, T. K. Allison, et al., Nature, 488,7413, 603, 2012.

[4] D. Popova-Gorelova, D. A. Reis, and R. Santra. Phys. Rev. B, 98, 224302, 2018.

[5] C. Orenelis-Skarin et al.,to be published.

This work was supported by the AMOS program within the Chemical Sciences, Geosciences, and Biosciences Division, U.S. Department of Energy.

[IL-06]

Advantage of Enzyme Structure Complexed with Cofactor using SFX: 3-Hydroxybutyryl-CoA Dehydrogenase from *F. prausnitzii A2-165*

S. Park†, J. Yang†, S. Jang, B. Shin, K. Bang, S. Kim, and K. Y. Hwang*

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Structure-based Drug Design (SBDD) is the process of creating and optimizing a chemical structure to find a molecule suitable for clinical testing, often known as a drug candidate. It is based on an understanding of the drug's three-dimensional structure and how its shape and charge interact with its biological target to produce a therapeutic effect (1, 2). As a result, when most scientists begin a drug discovery research project, they expect to have coordinates and associated electron density maps, as well as the ability to compare various structures of the same target protein or ligand (or small molecules). DeepMind's Alphafold3 AI algorithm predicts proteins' 3D structures based on their amino acid sequence. It consistently achieves accuracy comparable to experiment (3). However, thus far, this has frequently resulted in an error and one of the missing strategies. Given these factors, we need to get the reality check whether this structure is right data or not. As a result, it can effectively supply us with new insights for drug discovery. I'll show you three crystal structures complexed with small molecules in our lab and explain what they mean. In particular, we will discuss the progress of our recently solved '3HcoD-NAD-3HBtCoA complex structure using Serial Femptosecond Crystallography method at X-FEL/PAL'

References

1. Yoon IN et.al., Control of fibrosis with enhanced safety viaasymmetric inhibition of prolyl-tRNA synthetase 1. *EMBO Molecular Medicine* (2023)

2. Kim HT. et.al., Structural Basis for Inhibitor-Induced Hydrogen Peroxide Production by Kynurenine 3-Monooxygenase. *Cell Chem. Biol.*, (2018).

3. Jumper, J. et.al., Highly accurate protein structure prediction with AlphaFold, *Nature* (2021)

Acknowledgements

This work was supported by grants from the National Research Foundation of Korea (2020R1A2C2005670 and RS-202200143178) and Beamline X-FEL at Pohang Light Source.

[IL-07]

Experimental Studies of Water's Second Critical Point at PAL-XFEL

K. H. Kim*

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Water is the most important liquid for our existence on Earth and plays an essential role in physics, chemistry, biology, and geoscience. In the liquid form, water has numerous anomalous properties as compared to other liquids such as density maximum at 4-degree C. As an explanation for these anomalous experimental observations, a hypothetical liquid-liquid transition (LLT) and a liquid-liquid critical point (LLCP) has been proposed deep in the supercooled regime but has never been observed. Thus, the microscopic origin of the anomalous properties of water is elusive and there has been an intense debate for over a century.

Recently a new method of rapid cooling and ultrafast probing with wide-angle X-ray scattering (WAXS) using PAL-XFEL has allowed the venture into no-man's land and we found the first direct experimental evidence of the existence of the Widom line, LLT, and LLCP [1-2].

Reference

[1] K. H. Kim et al., “Maxima in the Thermodynamic Response and Correlation Functions of Deeply Supercooled Water”, Science, 358, 1589-1593 (2017).

[2] K. H. Kim et al., “Experimental Observation of the Liquid-Liquid Transition in Supercooled Water”, Science, 370, 978-982 (2020).

Abstract of Parallel Session

[PS-01]

Parallel Session: Ultrafast Photo-induced Dynamics in Condensed Matter at PAL-XFEL

Convener : Hoyoung Jang and Sae Hwan Chun

In this session, we intend to bring together researchers studying ultrafast photo-induced dynamics in condensed matter. We will review the current status of experimental setups at PAL-XFEL, discuss the ongoing research, and hear feedback from the users.

Agenda

1. Reviewing the PAL-XFEL setups for studying ultrafast photo-induced dynamics in condensed matter
   - Jaeku Park for Hard X-ray setups: Femtosecond X-ray Scattering (FXS)
   - Hoyoung Jang for Soft X-ray setups: Resonant soft X-ray Scattering (RSXS)

2. Young scientists' presentations: Ongoing research at PAL-XFEL
   - Time-resolved x-ray scattering study on polar vortex structure using XFEL
     by Kook Tae Kim (POSTECH)
   - Ultrafast lattice dynamics of $SrRuO_3$ and $SrRuO_3$-based superlattices
     by Dhawud Sabilur Razaq (Chungbuk National University)
   - Mapping free energy landscape in charge-ordered kagome metals using ultrafast X-ray diffraction
     by Seongyong Lee (POSTECH)

3. Open discussion and feedback

[PS-02]

Parallel Session: Exploring Chemical Reaction Dynamics with PAL-XFEL : A Symposium for Young Scientists

Convener : Jae Hyuk Lee and Sang Han Park

We're very excited to bring together young scientists working on ultrafast chemical reaction dynamics. We'll take a look at the current state of experimental setups at PAL-XFEL, such as time-resolved X-ray spectroscopy and time-resolved X-ray liquidography, and discuss ongoing research.

Agenda

1. Update of the beamline statue in the chemical science

2. Young scientists' presentations:
   - Development of hard X-ray spectrometer using polycapillary optics for XAS measurements of dilute samples at PAL-XFEL
     by Jinkyu Lim (Catholic Univ.)
   - Exploring structural dynamics of iodoform photolysis via time-resolved X-ray liquidography at PAL-XFEL
     by Yongjun Cha (KAIST)
   - Investigation of ligand charge delocalization mediated charge transfer on the bridged bimetalic complex
     by Junho Lee (KAIST)
   - Photo-induced spin cross-over dynamics in cytochrome c
     by Junwoo Bae (Mokpo National Univ.)

3. Open discussion and feedback

[PS-03]

Parallel Session: Basic Description and Discussion for Successful SFX Experiment

Convener : Sang Jae Lee

For this session, we aim to provide explanations and concepts pertaining to the apparatus used for SFX experiments, the processes involved in calculating a target structure, and Q&A addressing these topics.

Agenda

1. The status and fundamental description of equipment for SFX experiments.

2. Methods for structural calculations.

3. Interactive discussion and feedback

[PS-04]

Parallel Session: Femtosecond Time Resolved Imaging Experiment

Convener : Sunam Kim, Sangsoo Kim and Daewoong Nam

In this parallel session, discussions will be held on two imaging techniques based on the PAL-XFEL source: Bragg Coherent X-ray Diffraction and Dark Field Imaging. A brief explanation of the imaging techniques, principles and equipment will be provided. Afterwards, we will discuss the future direction of imaging techniques.

Agenda

1. The status and descriptions of techniques for femtosecond imaging experiments.
   - Bragg Coherent X-ray Diffraction Imaging @ XSS
   - Dark Field Imaging @ NCI

2. Open Discussion for future direction
   - New Users
     Director's- and Screening Beamtime
   - Joint Beamtime of Imaging Beamlines in PAL-XFEL and PLS-II

Abstract of Poster Presentation

[PP-01]

Ultrafast structural dynamics of I_2 in methanol visualized with femtosecond X-ray liquidography

J. Gu, J. H. Lee*, H. Ihee**

Department of Chemistry, Korea Advanced Institute of Science and Technology (KAIST), Daejeon 34141, Republic of Korea, *Pohang Accelerator Laboratory, Pohang, Gyeongbuk 37673, Republic of Korea, **Center for Advanced Reaction Dynamics, Institute for Basic Science (IBS), Daejeon 34141, Republic of Korea

The I_2 molecule in a solvent is a fundamental and crucial role in understanding how a solute behaves in a solvent environment and how chemical or physical interactions with the solvent influence the dynamic changes of the I_2 molecule. Owing to these advantages, the photoreaction dynamics of I_2 in various solvents have been extensively studied over the past few decades using techniques such as time-resolved spectroscopy and time-resolved X-ray scattering. However, there is a lack of studies monitoring the structural dynamics of I_2 in polar solvents on an ultrafast timescale. Here, we investigated the ultrafast structural changes of 400 nm excited I_2 in methanol using fs-XFEL, which offers superior time resolution. Upon excitation, the I_2 molecule exists briefly in an excited state with an I-I distance approximately 0.1 Å longer than the ground state for tens of femtoseconds. It then decays into two intermediates (3.9 Å and 4.8 Å) over the course of hundreds of femtoseconds. The intermediates decay to the ground state within hundreds of femtoseconds or splits into two I atoms within several picoseconds, respectively. The generated I radicals subsequently recombine over a few picoseconds. These findings are consistent with previous results in time-resolved spectroscopy. Research on the ultrafast structural changes of excited-state I_2 molecules in solution using fs-XFEL can serve as a useful guideline for future research.

[PP-02]

Understanding the Processes Occurring During an 800 nm Optical Laser Probe on Liquid Water

M. Ki, M. Shin, K. H. Kim

Department of Chemistry, Pohang University of Science and Technology, Pohang, 37673, Gyeongbuk, Korea

Water, one of the most abundant and versatile material on the planet, has studied intensely due to its anomalous properties. Although pump-probe experiment using optical laser as pump signal and XFEL source X-ray as pump successfully investigated rotational anisotropic signal of water induced by the laser pump, discussion on other possible processes such as multiphoton ionization are poorly done. Thus, herein, we report two distinct pump-probe time-resolved X-ray scattering experiments performed at FXL beamline at PAL-XFEL, varying laser fluence from 3 TW/cm2 to 168.53 TW/cm2 and its polarization. Simultaneously, two different sample of liquid water and deuterium oxide had been compared to confirm its nuclear quantum effect on rotational motion.

[PP-03]

Elucidating the effects of sulfur atoms on the photo-induced dynamics of thiouracils using time-resolved X-ray absorption spectroscopy

H. E. Oh, T. G. Woo, J. H. Lee, , R. R. Ma*, J. H. Lee*, T. K. Kim

Department of Chemistry, KAIST, Daejeon, 34141, Korea, *PAL-XFEL, Pohang, 37673, Kyungbuk, Korea

In heterocyclic thione molecules, a high-yield intersystem crossing is frequently observed, distinguishing them from their carbonyl analogs, which typically remain stable under UV/visible light irradiation. The precise role of the sulfur atom in causing these dynamic differences, however, has not been fully elucidated. In this study, femtosecond X-ray absorption spectroscopy at the sulfur K-edge was employed, combined with a 266 nm laser pump, to investigate the effects of the sulfur atom on photo-induced dynamics. The thiouracils in which one or two carbonyl groups were substituted by sulfur were examined, and their time-evolutions were meticulously compared. Early-time intersystem crossings which accelerated with an increasing number of sulfur substitutions were identified, and an additional relaxation component in the double-substituted systems was observed. Theoretical calculations predicted that the structure near the sulfur atom is heavily involved in the relaxation of excited states. By integrating experimental results with quantum chemical calculations, the overall dynamics at an orbital resolution were explained, correlating the changes in geometric and electronic structures.

[PP-04]

Photo-induced spin cross-over dynamics in cytochrome c

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Cytochrome c (cyt-c) is a metalloprotein with an iron-centered heme cofactor and plays a critical role to regulate an electron transfer in living organisms. The oxidized heme has a five-coordinated structure adopting the low spin state, and companies the geometric change upon the reduction of the heme cofactor from the external electron transfer. Even though such an interconversion process between oxidized, called as ferric state, and reduced cyt-c, called as ferrous state, is particularly vital to protein function, the detailed study in terms of spin state is elusive. In this study, we aim to investigate the photoinduced spin cross-over dynamics of ferric cyt-c in order to reveal the spin change of metal-center associated to the oxidation state. We conducted femtosecond X-ray absorption and emission spectroscopy (XAS & XES) experiments at the FXL beamline of PAL-XFEL. The time-resolved XAS results showed that the photo-excitation involves the ultrafast change of oxidation state with the formation of ferrous state. To scrutinize the spin state in the excited-state, we installed the XES setup based on a von Hamos spectrometer to acheive the highest energy resolution in the transient data. The XES results enables us to check the high-spin state such as quintet or triplet. This information will be further utilized for the future experiments to track the ultrafast spin dynamics in the XES data.

[PP-05]

Application of Single Object Scattering Simulation to Unveil the Fluctuating Structures of Biological Macromolecules

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Biological macromolecules are essential components of life, displaying dynamic structures in their natural environments. Traditional structure determination techniques often oversimplify these multifarious conformations by only capturing time-averaged molecular structures. In this work, we applied single-object scattering sampling (SOSS) technique to a diverse biological molecules. This "Bio-SOSS" technique utilizes ultrashort X-ray pulses to capture instantaneous structures. We use two gold nanoparticles (AuNPs), that provide strong contrast the X-ray scattering signal, as labels to enable precise distance measurements between labeled sites. We created hypothetical Bio-SOSS images of various biomolecules labeled with two AuNPs at specific positions, and evaluated the measured distances between these labels with the actual ones used to generate the simulated data. For a representative RNA (1KXK), the standard deviation of distance discrepancies was optimally around 0.2 Å and typically within 1 Å under practical experimental conditions at state-of-the-art X-ray free-electron laser facilities. Our study highlights the potential of Bio-SOSS for accurately capturing the diverse conformational spectrum of biological macromolecules, paving the way for deeper insights into their dynamic properties.

[PP-06]

Development of hard X-ray spectrometer using Polycapillary optics for XAS measurements of dilute samples at PAL-XFEL

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Time-resolved experiments with the advanced temporal/spatial resolutions of PAL-XFEL can give significant contributions to various fields of scientific research. Particularly, time-resolved X-ray absorption spectroscopy (XAS) with hard X-ray XFEL allows selective analysis of specific target elements (element selectivity) under *in-situ* conditions. Therefore XAS is widely used to track the changes on atomic or electronic structures of the samples. However, reliable XAS measurements of dilute samples are often challenging. Because, in the dilute conditions, the fluorescence signals irradiated from the sample are weak, while a significant amount of scattered photons are simultaneously detected, limiting our XAS capabilities.

To address this, we are developing a new hard X-ray XAS spectrometer. This novel XAS measurement setup will selectively deliver the fluorescence signals to the detector while suppressing scattering signals for reliable XAS measurement under dilute or scarce sample conditions. Polycapillary optics will be employed to collimate the emitted photons from a tiny interaction point into a beam size of around 2.5 cm. The collimated fluorescence photons will then be selectively deflected by a flat analyzer positioned at the Bragg position, ensuring only the sample's fluorescence is delivered to the detector. To secure high throughput, a graphite crystal will be used. We expect to achieve time-resolved XAS measurements of more than *x10* times dilute samples compared to current limitations at the Pt L3 edge.

This novel setup will allow easy alignments and energy changes. We hope it to be widely used for XAS measurements in various scientific research areas, such as time-resolved XAS analysis of heterogeneous materials like photocatalysts.

[PP-07]

Unveiling excited-state molecular dynamics of $Co(AcAc)_3$ using the combined probes of femtosecond X-ray and optical absorption spectroscopy; structural insight for hidden charge-transferred state

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Transition metal complexes (TMCs) have been widely studied due to their solar energy conversion ability and photonic applications. Excited-state potential energy surfaces and electronic behaviors in TMCs are directly associated with the rate of photoinduced charge transfer, which is one of the key factors in regulating macroscopic photocatalytic activities. To investigate the ultrafast electronic dynamics of metal-based photocatalysts, femtosecond X-ray spectroscopies have been developed using the X-ray pulse generated from an X-ray free electron laser (XFEL), instead of the optical pulse as a probe. X-ray probing pulse can provide chemical information about the local electronic and nuclear structures of the metal centers due to superb elemental specificity. Our study revealed that the fast structural distortion from Franck-Condon state to ^{1}LMCT occurred within 140 fs followed by intersystem crossing at the rate of 1.4 ps and longer lifetime constant which can be assigned to ^{3}MC. This study debunked the idea that the axially ligated reaction coordinate in this complex plays a critical role during the photoinduced charge transfer between the ligand and metal moieties. This ultrafast dynamics research on $Co(AcAc)_3$ molecule can facilitate the effective fabrication of TMC-based molecular photocatalysts by understanding early-time electronic and geometric changes caused by photo-induced charge transfer.

[PP-08]

Visualizing the Structural Change of a Metal−Organic Framework Using Femtosecond Serial Crystallography

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Time-resolved serial femtosecond crystallography (TR-SFX) is an experimental technique that combines the pump-probe scheme with serial femtosecond crystallography (SFX), allowing for the observation of ultrafast, damage-free structural changes in a crystal [1]. Still, the application of TR-SFX has been limited to protein samples. Here, we present the first TR-SFX study conducted on a non-protein sample, specifically a metal−organic framework (MOF) [2]. Our target sample is an iron-porphyrinic zirconium MOF known as porous coordination network−224 (PCN−224(Fe)) [3]. The Fe in the Fe porphyrin linker of PCN−224(Fe) can adsorb gas molecules such as CO. Upon photoexcitation, the adsorbed CO dissociates from the Fe, inducing an overall structural change in the MOF. Using TR-SFX, we visualized the dissociation of CO and the resultant structural changes in the MOF. Consequently, we identified three intermediates involved in the reaction and elucidated their kinetics and 3D structural changes. This study not only elucidates the detailed structural changes of PCN−224(Fe) upon photoexcitation but also lays the groundwork for expanding the application of TR-SFX to other systems, such as molecular crystals of small molecules.

[1] V. Šrajer and M. Schmidt, *J. Phys. D*: *Appl. Phys.*, 50, 373001 (2017)
[2] D. Feng *et al.*, *J. Am. Chem. Soc.*, 135, 17105 (2013)
[3] J. Kang *et al.*, *Nat. Chem.*, 16, 693 (2024)

[PP-09]

Elucidating the Melting Dynamics of Crystalline Ice on a Picosecond Timescale Using Time-resolved X-ray Scattering

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The melting of ice and the recrystallization of liquid water has been investigated intensively for the reason that water is one of the abundant and important substances for lives on Earth. However, the detailed mechanisms of ice melting in terms of structural dynamics were not fully elucidated despite the numerous studies using time-resolved optical spectroscopies and molecular dynamics simulation. By combining a rapid T-jump with an intense X-ray pulse from free-electron lasers (FELs) as a probe, we could elucidate the detailed structural dynamics of ice melting. To investigate the melting and recrystallization dynamics of crystalline ice I, we conducted a time-resolved X-ray scattering experiment in the time window from ns to μs. Using information extracted from the wide-angle X-ray scattering (WAXS) and small-angle X-ray scattering (SAXS) patterns, we estimated the time-dependent changes in the size and number of liquid domains, indicating that partial melting and superheating of ice occurs at around 20 ns. Following that, we recently explored the earlier stages of dynamics with the wider time window (ps~us) and found interesting melting/recrystallization features on the ps and ns timescales, by analyzing the SAXS and WAXS patterns.

[PP-10]

Investigation of Ligand Charge Delocalization Mediated Charge Transfer on the bridged bimetalic complex

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Understanding the charge transfer mechanism of the donor-acceptor system is a long-term topic of investigation in the chemist society. In the bridged bimetallic donor-acceptor complex, the ligand charge delocalization in the Metal-to-Ligand Charge Transfer (MLCT) state plays a significant role in the charge transfer between two metal centers. In ths work, we employed site-specific femtosecond metal L_3-edge X-ray absorption spectroscopy (XAS) to probe the light-induced charge transfer process in the tetrapyridophenazine-bridged Ru(II)/Os(II) complex at each metal center seperately. The slight deceleration of the charge delocalization and early depopulation in the MLCT state at the electron-accepting Ru(II) center introduced by the opposite Os(II) is observed. Meanwhile, the acceleration of the charge delocalization process in the MLCT state centered at the electron-donating Os(II) center is observed. Moreover, combined with theoretical calculations and Os L_3-edge XAS, we possible to probe that the elongation of metal and bridging ligand distance is mediated by the ligand charge delocalization. Our study shows that the excited state dynamics at one metal center are significantly affected by the opposite metal center, and the ligand charge redistribution is strongly correlated with the metal and bridge ligand distance.

[PP-11]

Efficient Conversion of Methane to Ethanol with Fe Single Atom Catalysts

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We introduce a new method for converting methane to ethanol using Fe single-atom catalysts. These catalysts effectively stabilize oxygen, eliminating the need for oxygen evolution reactions and improving ethanol production efficiency. To analyze the local coordination environment of Fe SAC, X-ray absorption near-edge structure (XANES) and extended X-ray absorption fine structure (EXAFS) are utilized. Our computational study reveals an optimal zone for maintaining active oxygen on Fe single-atom catalysts, with the formation of oxyhydroxide intermediate being a key step. We describe a straightforward process where methane is directly oxidized to methanol, then converted to ethanol. Additionally, we've used a direct gas diffusion flow cell to better transfer methane, significantly enhancing conversion efficiency. This method showcases the potential of Fe single-atom catalysts for sustainable ethanol production from methane.

[PP-12]

X-ray Absorption Spectroscopic Analysis and Phase Engineering of Lepidocrocite-Type Titanate/NiCo-LDH Heterostructured Electrodes

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This study proposes a novel electrode material development approach based on surface charge storage mechanisms, achieved through the partial phase change of heterojunctions utilizing two-dimensional layered materials. To maximize surface charge storage reactions beyond the crystallographic theoretical capacity, we synthesized heterojunctions composed of chemically exfoliated transition metal oxide nanosheets (Lepidocrocite-Type Titanate, Nickel-Cobalt Layered Double Hydroxide) and controlled the phase change to induce various polymorph formations. The crystallographic mismatch of transition metal oxide nanoparticles derived from two-dimensional nanosheets promotes the formation of rich grain boundaries, providing accessible surface storage sites for Li-ions. Moreover, the surface storage mechanism at the nano-interfaces maintains excellent structural stability even after long-term cycling, as it does not alter the internal crystal structure, enabling high-rate charging/discharging due to its diffusion-independent characteristics. These phase-changed compounds exhibit entirely different crystal and local structure tendencies than conventional layered materials. Therefore, we elucidated the oxidation state and local structure of phase-changed materials by synchrotron X-ray absorption spectroscopic analysis.

[PP-13]

Role of Cations to Charge Density Wave in Kagome Metal via Time-resolved X-ray Diffraction

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The vanadium-based kagome metal, AV3Sb5 (A=K, Rb, Cs), exhibits significant effects of A-site cations on the Charge Density Wave (CDW) phase and superconductivity. Utilizing X-ray diffraction, CDW structures and CDW phase transition temperature of RbV_3Sb_5 were identified. Moreover, through time-resolved X-ray diffraction, we examined the influence of A-site cations on the CDW phase in RbV3Sb5. This revealed contrasting dynamics between 2×2×1 and 2×2×2 CDW orders after the photoexcitation of conduction electrons near the Fermi surface. Especially, the 2×2×2 CDW order exhibited complex behavior involving coherent phonon linked to the A-site cation's displacement. And 2×2×2 CDW coherent phonon oscillation was π shifted with respect to DECP simulation. These findings offer strong support to the hypothesis that A-site cations significantly impact the 2×2×2 CDW phase in RbV_3Sb_5.

[PP-14]

Ultrafast lattice dynamics of $SrRuO_3$ and $SrRuO_3/SrTiO_3$ superlattices

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$SrRuO_3$ (SRO) has strong couplings among lattice, charge, and spin degrees of freedom, which manifest themselves in temperature dependent evolutions of resistivity and lattice constants across the magnetic transition temperature (TC ~160 K). The structural symmetry of $SrRuO_3$ can also be systematically controlled in $SrRuO_3/SrTiO_3$ heterostructures by varying the thickness of adjacent $SrTiO_3$ (STO) layers.

In this work, we investigated the lattice dynamics of SRO/STO superlattices and a SRO film using an optical pump and x-ray probe method. It is known that femtosecond pulse excitation of SRO induces an ultrafast lattice expansion. The transient X-ray intensity of superlattice satellite peaks of superlattices upon pumping shows oscillatory behavior. The oscillation frequency corresponds to zone-folded acoustic phonon mode of the superlattices. At room temperature, the peak intensity increases upon pumping, which is attributed to the expansion of the SRO layer. However, in the magnetic state (<130 K), the intensity decreases upon pumping in the low fluence limit, indicating compression of the SRO layer. As the pump fluence increases, the oscillation phase shows a gradual change, revealing evolution from the photo-induced lattice compression in the low fluence condition to the expansion in a high fluence case. The unique ultrafast lattice dynamics is attributed to the magnetostriction of SRO in the magnetic state competing with the thermal expansion. Detailed investigation on various Bragg peaks of a SRO single layer film suggests that a specific lattice distortion is responsible for the ultrafast lattice dynamics of SRO.

[PP-15]

Time-resolved RIXS and quantum materials

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Quantum materials have been deeply studied due to their scientific interest. Many researchers have tried to find new insights and intriguing material systems, such as antiferromagnet-based spintronics and energy conversion in transition metal oxides. In particular, the Ir 5d orbital states of IrO2 and other iridates can play an important role in the energy conversion process and the spin-orbit entangled systems. However, understanding of the process of the model system is yet incomplete due to experimental limitations.

Here we tried to develop an experimental approach based on time-resolved resonant x-ray inelastic scattering at the Pohang Accelerator Laboratory X-ray Free electron facility (PAL-XFEL), which has been used to systematically elucidate new properties of quantum materials such as iridates. We aimed to provide theoretical guidelines for advanced hard x-ray scattering techniques. We propose that this approach can explore intriguing dynamics and unveil the energy conversion process.

[PP-16]

Photo induced ultrafast phase-transition of metallic glass directly observed by single-pulse imaging with XFEL

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The exploration of ultrafast light-matter interactions has invigorated research on light-induced quantum control of material properties by opening new avenues for producing new phases of matter in nonequilibrium states. In this study, we investigate ultrafast melting of metallic glass materials using time-resolved single pulse imaging. The metallic glass exhibits an amorphous structure without long range atomic orders. The absence of crystalline order gives rise to distinctive melting reactions. Its melting process is expected to be different from the crystalline metal as the absence of phonons. However, the fundamental mechanisms underlying the rearrangement of the metallic glass structure remain elusive. By conducting the single-pulse time-resolved imaging experiments performed at PAL-XFEL, we obtained direct nanoscale images of single metallic glass nanoparticles (MG-NP) undergoing nonequilibrium melting excited by femtosecond IR laser (800 nm). Upon laser illumination, anisotropic shape deformation of the MG-NP occurred promptly (within 1 ps). The NP deforms, accompanied by an inhomogeneous distribution of the mass density, more severely as the melting proceeds. Inhomogeneity in the density distribution becomes more apparent. It displays highly inhomogeneous distribution with low-density regions localized to form bands, which prevents further development of shape deformation. We present the nanoscale imaging results that visualize ultrafast melting in metallic glasses, which promote in-depth understanding of structural deformation accompanied during the melting (glass) transition.

[PP-17]

Time-resolved Ultrafast Strain Evolution in $SrTiO_3$ Nanocrystals by Bragg Coherent X-ray Diffraction Imaging

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The formation of polarons and relevant deformations in atomic displacement in perovskite-oxides is due to the localization of charged carriers within photo-excited crystal lattices. It is important to understand these phenomena and processes in an ultrafast time scale for practical applications and the underlying science because such a polaron affects structural distortions and carrier transport in perovskite-oxides. Additionally, the deformation caused by these excited carriers can induce ferroelectricity in $SrTiO_3$. Perturbations that induce this ferroelectricity include strain, doping, and defects, and it is also reported that polarons and resonant bonding induced by light can cause it. In the equilibrium state, the TO1 phonon mode is associated with phase transition, but the light-induced ferroelectricity involves the LO2 and LO3 phonon modes, which are considered a non-thermal process. This ferroelectricity is typically referred to as a "hidden" state in $SrTiO_3$, different from the state formed in equilibrium, and it has been confirmed through calculations to be transiently reached. Using the BCDI technique at XFEL, we observed the induced polarons and the resulting displacive transient ferroelastic transition in $SrTiO_3$ nanoparticles excited with above band-gap energy. This transition was confirmed by BCDI results, showing that strain forms a stripe pattern starting at around 4 ps. This deformation continued to evolve up to about 20 ps, as confirmed by XRD patterns. Our results are expected to provide a comprehensive understanding of ferroelectric polarons, where polarons formed by excited carriers transition into ferroelectricity. This work was supported by the National Research Foundation of Korea grant NRF- 2021R1A3B1077076.

[PP-18]

Ultrafast DFXM for Light-Induced Structural Evolution

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DFXM (Dark-field X-ray Microscopy) has recently gained attention as a promising research method for clearly visualizing domains and defects within materials. The principle feature of DFXM is its ability to produce real-space images of domains selected by the orientation of the Bragg peak using an objective lens. Additionally, DFXM at XFEL facilities is notable for enabling time-resolved dynamics studies in conjunction with femtosecond laser pumping. One of these dynamics studies focuses on understanding the behavior of surface scattered waves and shock waves induced by lasers. This understanding is crucial not only for material applications but also for advancing the fundamental understanding of solid-state physics. In this presentation, I will discuss the behavior of scattered waves on the topological 2D material Bi_2Se_3 and Cu film surface induced by fs-laser. Both bulk crystal maintains strong crystallinity up to the surface, resulting in very clear DFXM results. Based on tests with approximately X-ray 1000 shots, we found that internal domains do not change in response to X-ray shots. However, a single laser shot generates transient surface scattered waves around 20 ps. As the laser fluence increases, the spacing of the ripple pattern decreases. We also observed that changes in the laser wavelength have little effect. These surface ripple patterns were found to form across domain boundaries on the surface. However, it was also observed that waves reflect at boundaries close to the surface. While surface scattered waves are considered to be caused by surface plasmon polaritons, other influences are also inferred to be present. In the case of Cu, we successfully observed both surface scattered waves and shock waves. From 10 ns, shock waves were observed with a speed measured at approximately 6 km/s, which is close to subsonic speeds. This work was supported by the National Research Foundation of Korea grant NRF- 2021R1A3B1077076.

[PP-19]

Void Nucleation in Ultrafast Photoinduced Melting Revealed by Time-Resolved Coherent Diffraction Imaging

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The interest in ultrafast light-matter interaction has increasing significantly with the availability of femtosecond laser pulses to enable mode-selective perturbation by exclusively exciting valence electrons. This has enabled researchers to track intermediate states during cascading reactions of energy transfer processes from optical excitation to eventual phase change of materials. We are revisiting the solid-liquid phase transition, with direct visualization, to gain an understanding of a fundamental physical phenomenon. Using single-shot XFEL time-resolved coherent diffraction imaging, we observed the direct density change on the femtosecond laser driven nonequilibrium dynamics of gold nanoparticles. By imaging laser fluence and polarization dependent atomic density distributions combined with all-atom simulations of two-temperature molecular dynamics, we uncovered that ultrafast melting of Au is controlled by photoexcited electron-originated transient ionic pressure. By filling the gap in understanding the dynamic interaction between electron and ion, this work provides a leverage to control ultrafast ionic dynamics with the femtosecond laser field.

[PP-20]

XFEL beam profile examination for tr-BCDI experiment

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Bragg coherent X-ray diffraction imaging (BCDI) technique represents its uniqueness from the coherence of the X-ray beam and the Fourier relation between the crystalline sample within the beam size and the respective diffraction patterns. The advantage of this technique is visualization of internal strain field without sample destruction. However, in order to fully utilize the aforementioned advantages, the stability of the incident X-rays must be guaranteed. From the perspective of selecting an X-ray source, the synchrotron source provides stability of the beam in intensity and beam position, there are disadvantages in absolute beam flux and the degree of spatial (transverse) coherence. X-ray free electron laser (XFEL) source gives opposite advantages and disadvantages from the synchrotron source, that gives high beam flux and almost complete transverse coherence in the scale of sample size, since there are fluctuations of beam positions and intensity. Thus, performing the BCDI technique on an XFEL source must be preceded by an evaluation of beam quality. In this study, we performed the BCDI experiment with gold nanoparticles in PAL-XFEL facility and subsequent analysis related to the beam quality factors. Through this, we aim to represent that the PAL-XFEL facility is suitable for conducting BCDI experiments.

[PP-21]

Simulation, fabrication, and performance test of Low Gain Avalanche Detector for X-ray detection

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A low gain avalanche detector (LGAD) provides a good timing resolution and moderate charge multiplication with an improvement of signal to noise ratio. Thus, the LGAD is studied as a device for a direct detection of X-ray. The Technology Computer-Aided Design (TCAD) simulation is performed to obtain fabrication and photomask design parameters. Considering an absorption length of X-ray and a mobility of carrier for easier charge multiplication, 400 μm-thick p-type silicon wafer with a high resistivity (8-10 kΩ·cm) is chosen. The LGAD sensor has basically Positive-Intrinsic-Negative (PIN) structure and a reverse bias voltage is applied for using a full depletion layer. There is a multiplication layer (P-well) underneath the N+ junction layer. The fabrication parameters, such as doping concentration, energy, annealing time, etc., obtained from TCAD simulation for these implants should be precisely controlled and optimized to achieve the desired gain value. To make the uniform electric field at the edge of the N+ implant, an additional highly doped region, known as the Junction Termination Extension (JTE), is considered. In this study, we present the simulation and mask design for fabrication, as well as performance test results, including electrical characteristics and gain test using an Sr-90 radioactive source, of the fabricated LGAD sensor.

[PP-22]

Time-resolved Hard X-ray Emission Spectroscopies using Self-seeded Pulses at PAL-XFEL

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The Pohang Accelerator Laboratory X-ray Free-Electron Laser (PAL-XFEL) has successfully generated self-seeded X-ray pulses via forward Bragg diffraction using a diamond monochromator across a wide photon energy range of 3.5 to 14.6 keV. The PAL-XFEL has applied a coordinated scanning scheme involving electron bunch energy, diamond crystal angle, and silicon monochromator, ensuring reliable energy scans. Harnessing self-seeded pulses with energy tunability at the PAL-XFEL, we conducted commissioning experiments of resonant X-ray emission spectroscopy (RXES) and time-resolved high-energy-resolution fluorescence-detected X-ray absorption spectroscopy (HERFD-XAS). A point-to-line von Hamos geometry for Ir $L\beta_2$ fluorescence from IrO_2 powder and a point-to-point Johann geometry for Cu $K\alpha_1$ fluorescence from $[Cu(dmphen)_2]^+$ in acetonitrile (dmphen = 2,9-dimethyl-1,10-phenanthroline) were aligned for each experiment. The incident photon energy was scanned with an energy step of 0.3 eV across the Ir L_3-absorption edge over 30 eV, and the Cu K-absorption edge over 60 eV, respectively. These two examples benefit from the self-seeded pulse with more than 10^{11} photons and a narrow bandwidth of ~0.5 eV in full width at half maximum. In this presentation, we show further details of both commissioning results and discuss available experimental schemes and parameters for user service.

[PP-23]

Current status of the CXI endstation for revealing structural information at nanoscale resolution

Daewoong Nam, Sangsoo. Kim, Sae Hwan Chun,
Intae Eom and Tae Yeong Koo

XFEL Beamline Department, Pohang Acclerator Laboratory, Pohang University and Science and Technology, Pohang 37673, Korea

In this presentation, we will introduce experimental equipment for X-ray imaging and describe its capability to reveal structural information of specimens at nanoscale resolution. The CXI endstation offers a unique opportunity to visualize ultrafast phenomena with nanoscale spatial and picosecond temporal resolution.

[PP-24]

Hard X-ray FXS instrument for the study of energy and quantum materials

Sae Hwan Chun

PAL-XFEL Division, Pohang Accelerator Laboratory,
POSTECH, Pohang, Gyeongbuk 37673, Republic of Korea

Research on energy materials and quantum materials has garnered significant interest in the fields of condensed matter physics and materials science due to their potential impact on everyday life, particularly in the areas of energy storage/conversion/transportation, and emergent functionality, respectively. In this presentation, I will provide an overview of the Femtosecond X-ray Scattering (FXS) instrument at the hard X-ray beamline of the PAL-XFEL and its applications in researching energy and quantum materials. The FXS instrument offers a wide range of X-ray probes, from basic X-ray diffraction to state-of-the-art resonant X-ray scattering. These probes are capable of capturing intriguing out-of-equilibrium states involving charge, spin, orbital, and lattice physical degrees of freedom. I will also discuss the current status of this instrument and directions for future development.

[PP-25]

Introduction to tr-BCDI system at XSS beamline

J. Kang, J. Park, S. Kim

XFEL Application Team, PAL-XFEL, POSTECH
80 Jigokro-127-beongil, Nam-gu, Pohang, Gyeongbuk 37673, Korea

X-ray Scattering and Spectroscopy (XSS) beamlineinPAL-XFELis developed for hard x-ray scattering and spectroscopy experiments. Time-resolved Bragg coherent x-ray diffraction imaging (tr-BCDI), a very specific imaging technique based onx-ray scatteringis also suitable through this beamline. Main experimental instrument consists ofx-rayoptics, 4-circle goniometer, 0.5mega pixel Jungfraudetector, and pump laser system. In this poster, detaileddescription of the instrument, experimental procedure, and feasiblesciences will be discussed.

[PP-26]

Laser systems for time-resolved experiments at Pohang Accelerator Laboratory X-ray Free-Electron Laser

Dogeun Jang, Minseok Kim, Gwangryeol Park, Hyeongi Choi, Intae Eom

Pohang Accelerator Laboratory, Pohang, Gyeongbuk 37673, Republic of Korea

Optical laser systems for ultrafast X-ray sciences have been established at the Pohang Accelerator Laboratory X-ray Free-Electron Laser (PAL-XFEL) beamlines. Three Ti:regenerative amplifier systems are synchronized with the XFEL with femtosecond precision. The low temporal jitter of the PAL-XFEL provides an experimental time resolution below 150 fs (full width at half-maximum). Fundamental waves, their harmonics, and tunable sources from ultraviolet to near-infrared, all with femtosecond pulse durations, are available for all beamlines. Additionally, tunable sources with nanosecond pulse durations are provided for one beamline. The position stability of the optical laser, determined by the intensity-based center of mass at the sample position, is less than 3% (r.m.s.) of the spot size. Through this presentation, we aim to introduce the comprehensive optical laser systems operated and utilized for ultrafast XFEL pump-probe experiments at the PAL-XFEL beamlines.

[PP-27]

Resonant Soft X-ray Scattering (RSXS) Endstation at PAL-XFEL

Hoyoung Jang, Gyeongbo Kang

XFEL Beamline Division, PAL-XFEL, Pohang Accelerator Laboratory, POSTECH, Pohang, 37673, Gyeongbuk, Korea

The Resonant Soft X-ray Scattering (RSXS) Endstation at the PAL-XFEL of the Pohang Accelerator Laboratory is under user operation since 2020. This endstation provides 400 – 1300 eV X-ray probe pulses and 250 – 2600 nm optical pump pulses with a time resolution of ~100 fs and 60 Hz maximum repetition rate [1]. The main research topics at the RSXS Endstation is photoinduced dynamics of quantum materials and magnetic materials. In addition to the resonant X-ray scattering technique, fluorescence-yield X-ray absorption spectroscopy and even nonresonant X-ray scattering are employed to investigate the optically excited solid materials.

In this presentation, the current setup of the RSXS Endstation is introduced. Moreover, I would like to present the scientific opportunities at the RSXS Endstation by introducing previous results. The results include the spectroscopy and scattering experiments of superconducting cuprates [2-4], the observation of coherent magnon in hexaferrites [5,6], and charge density wave dynamics in quasi-2D materials.

[1] Hoyoung Jang *et al.* Rev. Sci. Instrum. **91**, 083904 (2020).
[2] Denitsa R. Baykusheva *et al.* Phys. Rev. X **12**, 011013 (2022).
[3] Hoyoung Jang *et al.* Sci. Adv. **8**, eabk0832 (2022).
[4] Martin Bluschke *et al.* Proc. Natl. Acad. Sci. U.S.A. **121**, e2400727121 (2024).
[5] Hiroki Ueda *et al.* Phys. Rev. Research **4**, 023007 (2022).
[6] Hoyoung Jang *et al.* Adv. Mater. **35**, 2303032 (2023).

[PP-28]

A fascinating research platform for biology: Serial femtosecond crystallography endstation

Jaehyun Park, Sang Jae Lee, Sehan Park

PAL-XFEL, Pohang Accelerator Laboratory, POSTECH

Unveiling macromolecular structures in the ground states and fast motions become a key to understand various biological phenomena. The information of a three-dimensional electron density distribution in an atomic resolution significantly contributes to that purpose. The macromolecular crystallography is a conventional technique to retrieve the information through the X-ray diffraction experiments with crystalized samples. However, it has limitations on the several issues such as crystal size, cryo-temperature, and radiation damage. Serial femtosecond crystallography (SFX) is an emergent and popular technique to overcome the issues at the X-ray Free Electron Lasers (XFEL) facilities in the world. To perform the SFX, micro crystal delivery systems and sample chambers play important roles through maintaining perfectly hydrated environment to have the micro crystals in a stable condition. Here, we present about the current status of the SFX endstation established at the PAL-XFEL. The uniquely developed crystal delivery systems including liquid flow and fixed target methods will be introduced based on the features, specifications etc. (for instance, particle solution delivery (PSD) injector, carrier matrix delivery (CMD) injector, micro-liter volume (MLV) syringe injector, 2D fixed target, and the 1D fixed target). In addition, the specially designed sample chambers to operate various crystal delivery techniques and applicable sciences based on the systems will be explained with scientific cases performed at the PAL-XFEL.

[PP-29]

Latest developments in at XAS/XES endstation

Sang Han Park

XFEL beamline division, Pohang Accelerator Laboratory,

The Soft X-ray Scattering and Spectroscopy (SSS) beamline provides the XFEL with an energy range of 0.25 to 1.2 keV at a repetition rate of 60 Hz, with a pulse width as short as 90 fs. The SSS experimental instruments are designed for a variety of scientific programs, including those in physics, chemistry, and materials science, focusing on spectroscopy and scattering. The beamline comprises offset mirrors, a varied line spaced grating monochromator, and Kirkpatrick-Baez (KB) refocusing optics.

The experimental instruments of the XAS/XES endstation on the SSS beamline support a diverse range of scientific programs related to spectroscopy and coherent forward scattering, including imaging. Various experiments with different sample conditions can be conducted independently in the vacuum chamber, utilizing different detectors.

In this presentation, we will introduce the recent developments of the XAS/XES endstation on the SSS beamline.

[PP-30]

Studying of the Chemical Reaction Dynamics at Femtosecond X-ray Liquidography (FXL) Endstation

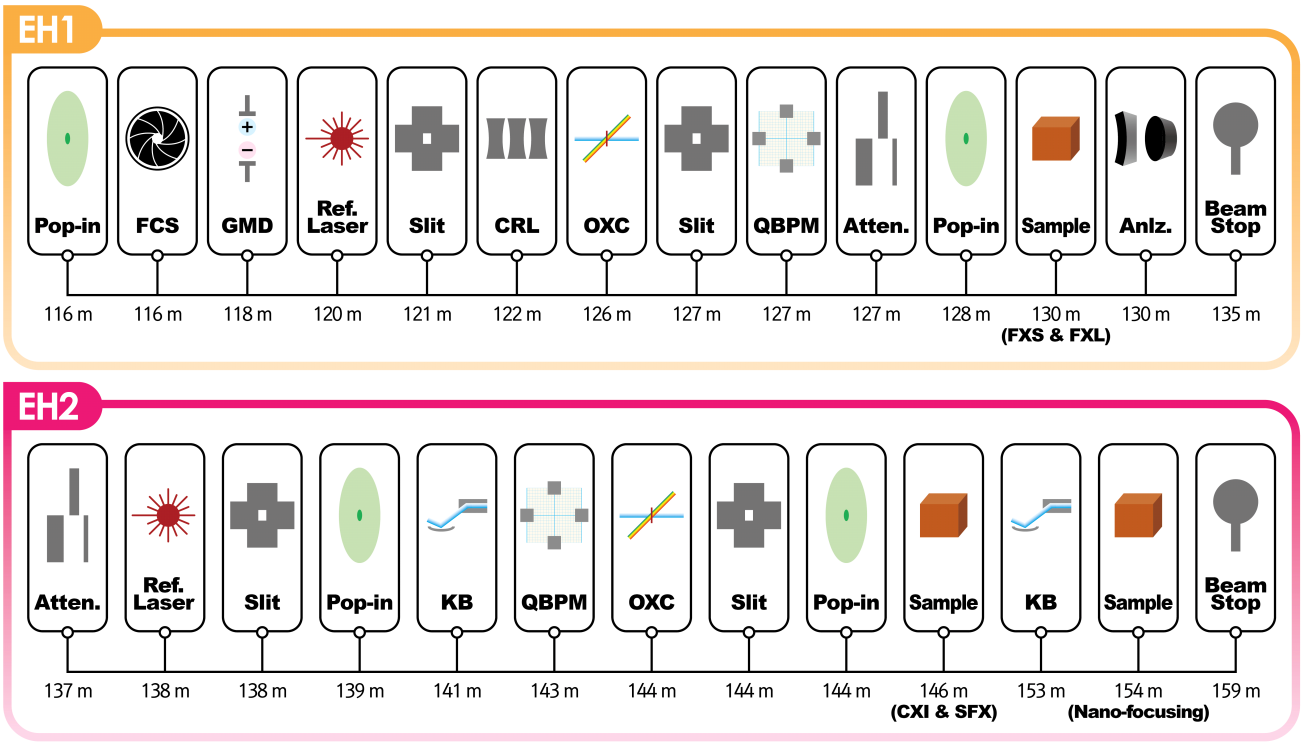
Jae Hyuk Lee, Rory Ma

XFEL beamline, PAL, POSTECH, Pohang, Kyungbuk, Korea

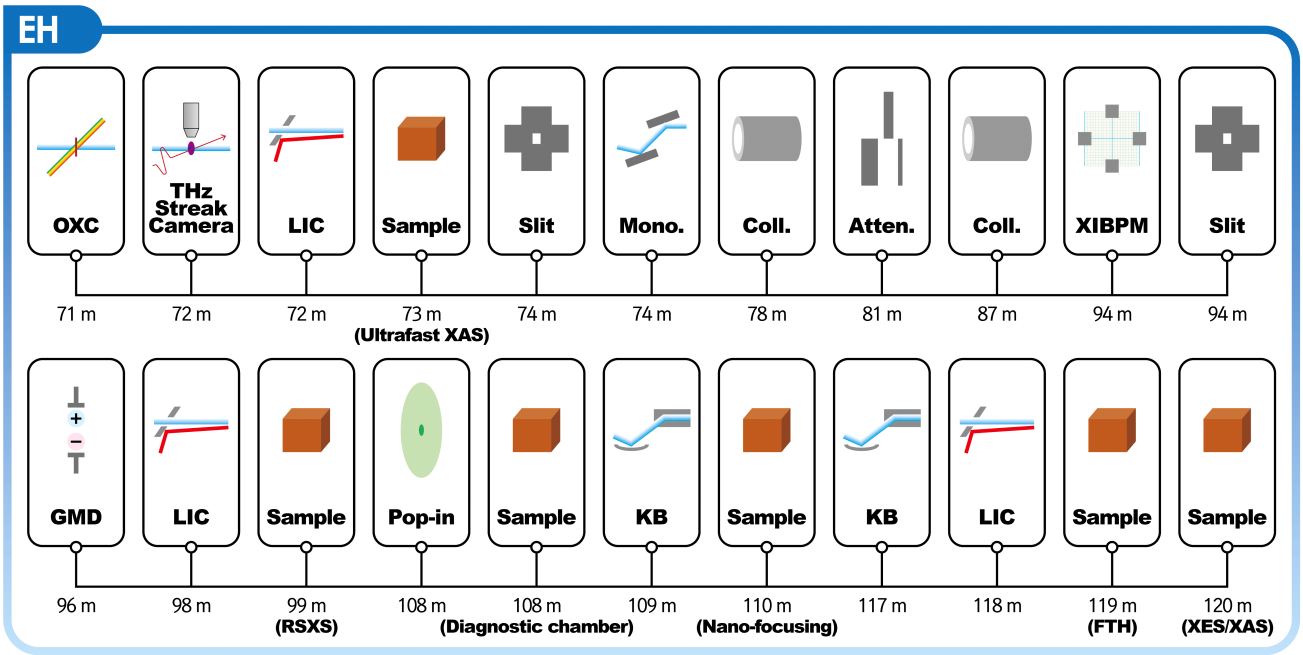
The femtosecond X-ray Liquidography (FXL) endstation at the hard X-ray scattering and spectroscopy (XSS) beamline in PAL-XFEL (Pohang Accelerator Laboratory's X-ray Free Electron Laser) commenced user service in June 2017. The objective of the FXL endstation is to track the chemical reaction dynamics occurring in various environments using XFELs. In the X-ray energy range of 2.3 to 20 keV, the primary experimental techniques employed by FXL are time-resolved X-ray solution scattering (liquidography) and time-resolved X-ray absorption and emission spectroscopy. The X-rays from PAL-XFEL have an extremely high brightness, with a flux of approximately 10^{12} photons per pulse at 9.7 keV and a duration of less than 50 femtoseconds. The combination of a femtosecond optical laser with XFEL enables the observation of ultrafast changes in the course of chemical reactions.

Supplementary Materials
PAL-XFEL Layout and
Summary for Experimental Setups

Hard X-ray Beamline



Soft X-ray Beamline

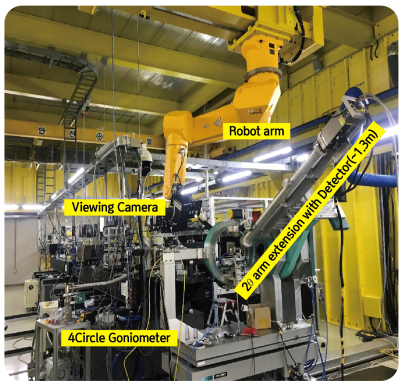


HX EH1 (XSS)

Femtosecond X-ray Scattering (FXS) Endstation

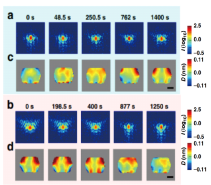
Experimental parameters

Laser incident angle	⟨10° (Vertical & Horizontal)
Laser wavelengths	240 nm – 2600 nm (800 nm harmonics, OPA)
Laser pulse duration	~40 fs (@800 nm)
Sample motion	6-axis (3 rotations + 3 translations)
Sample environment	~40 K (Cryostream) – 400 K (Heating System)
Detector	Jungfrau 0.5M



Scientific cases

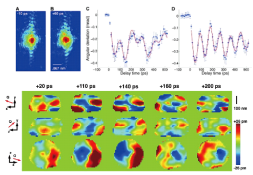
Solution for Climate Crisis



In-situ Visualization of Strain Field Inside of Zeolite Nanocrystal During Catalytic Chemical Reaction

J. Kang *et al., Nat. Comm.* **11**, 5901 (2020)

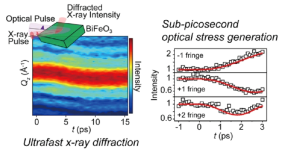
Image of Atomic Motion



In-situ 3D Visualization of Strain Field Inside of Au Nanocrystal Stimulated by Pulse Laser

J. N. Clark *et al., Science* **341**, 56 (2013)

Interaction of Light and Condensed Matters



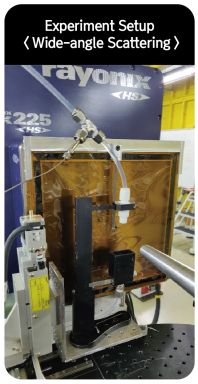
Subpicosecond Optical Stress Generation in Multiferroic $BiFeO_3$

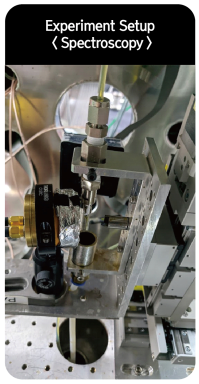
H. Lee *et al., Nano Lett.* **22**, 4294 (2022)

Femtosecond X-ray Liquidography (FXL) Endstation

Experimental parameters

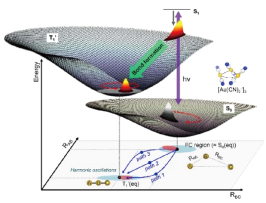
Laser incident angle	Collinear / 10°
Laser wavelengths	240 nm – 2600 nm (800 nm harmonics, OPA)
Laser pulse duration	~40 fs (@800 nm)
Sample environment	Liquid phase
Detector	Rayonix MX225-HS (WAXS) APD, Jungfrau 0.5M (Spectroscopy)





Scientific cases

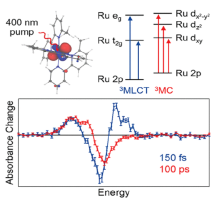
Capturing the Coherent Vibrations



Mapping the Emergence of Molecular Vibrations Mediating Bond Formation

J. G. Kim *et al., Nature* **582**, 520 (2020)

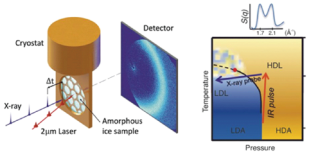
Tender X-ray Spectroscopy



Ligand-Field Effects in a Ruthenium (II) Polypyridyl Complex Probed by fs X-ray Absorption Spectroscopy

Y. Kim *et al., J. Phys. Chem. Lett.* **12**, 12165 (2021)

Liquid-Liquid Transitions Under Pressure



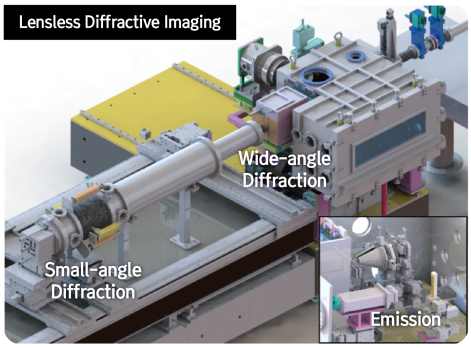
Experimental Observation of the Liquid-Liquid Transition in Bulk Supercooled Water Under Pressure

K. H. Kim *et al., Science* **370**, 978 (2020)

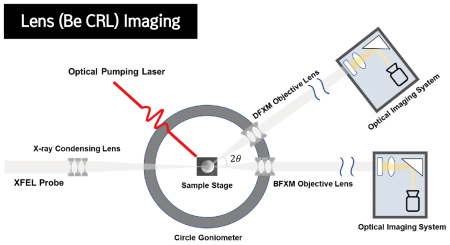
HX EH2 (NCI)

Coherent X-ray Imaging (CXI) Endstation

Lensless Diffractive Imaging



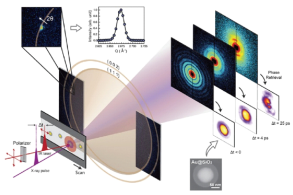
Lens (Be CRL) Imaging



BFXM (Bright Field XM) : transmission mode
DFXM (Dark Field XM) : reflection mode

Scientific cases

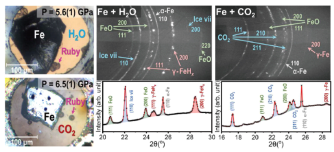
Coherent X-ray Imaging



Ultrafast Energy Transfer Process in Confined Gold Nanospheres

J. Shin *et al.*, *Nano Lett.* **23**, 1481 (2023)

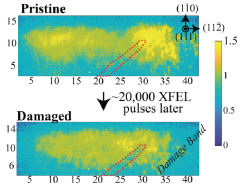
WAXS (Wide-Angle X-ray Scattering)



Oxidation of Iron by Giant Impact and Its Implication on the Formation of Reduced Atmosphere in the Early Earth

J. Choi *et al.*, *Sci. Adv.* **9**, eadi6096 (2023)

DFXM Imaging of Strain Waves



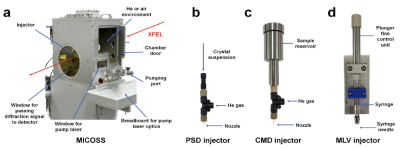
Visualization of Radiation Damage of Diamond Crystal

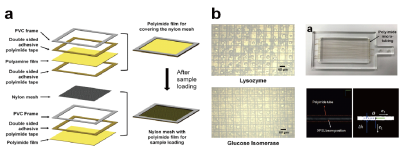
L. E. Dresselhaus-Marais *et al.*, *Sci. Rep.* **13**, 17573 (2023)

Serial Femtosecond Crystallography (SFX) Endstation

Experimental parameters

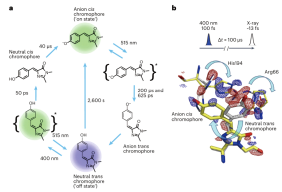
Laser incident angle	15° (collinear geometry to be added in the future)
Laser wavelengths	ns-laser: 210 nm – 2600 nm (OPO) fs-laser: 240 nm – 2600 nm (800 nm harmonics, OPA)
Laser pulse duration	~40 fs (@800 nm)
Sample delivery Sample environment	PSD, CMD, MLV injectors, fixed target MICOSS, FT chamber, Ambient system
Detector	Rayonix MX225-HS, Jungfrau 4M





Scientific cases

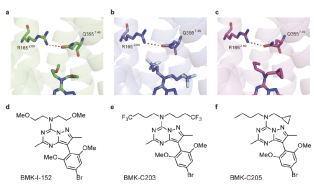
Optical Control of Ultrafast Dynamics



Optical Control of Ultrafast Structural Dynamics in a Fluorescent Protein

C. D. M. Hutchison *et al.*, *Nat. Chem.* **15**, 1607 (2023)

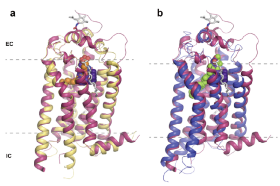
Drug Discovery



Structure-Based Drug Discovery of a Corticotropin-Releasing Hormone Receptor 1 Antagonist

H. Kim *et al.*, *Exp. & Mol. Med.* **55**, 2039 (2023)

Membrane Protein Structures



Structural Basis for Receptor Selectivity and Inverse Agonism in $S1P_5$ Receptors

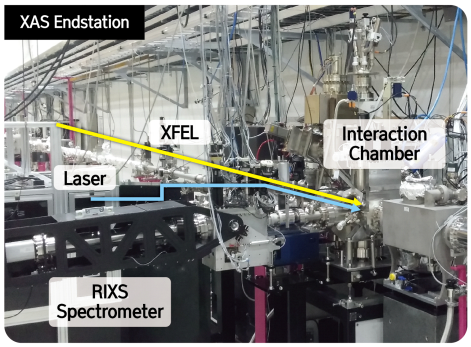
E. Lyapina *et al.*, *Nat. Comm.* **13**, 4736 (2022)

SX (SSS)

XAS/XES/FTH Endstation

Experimental parameters

Laser incident angle	Collinear (<1°)
Laser wavelengths	240 nm ~ 2600 nm (800 nm harmonics, OPA)
Laser pulse duration	~40 fs (800 nm)
Sample motion	5-axis (2 rotations + 3 translations)
Sample temperature	Down to ~25 K (LHe) or ~90 K (LN_2)



Scientific cases

Dynamics of Charge Carriers

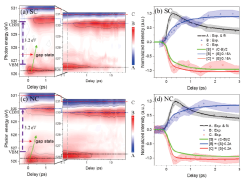
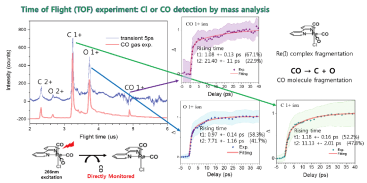


Photo Excited Carrier Dynamics for Electrons and Holes in TiO_2

S. H. Park, *et al.*, *Nat. Comm.* **13**, 2531 (2022)

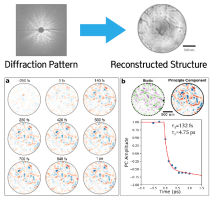
Dynamics of Chemical Reactions



Photolysis Dynamics of CO from Re-Complex

In Preparation

Change of Nano-Size Material in Resonant Energy



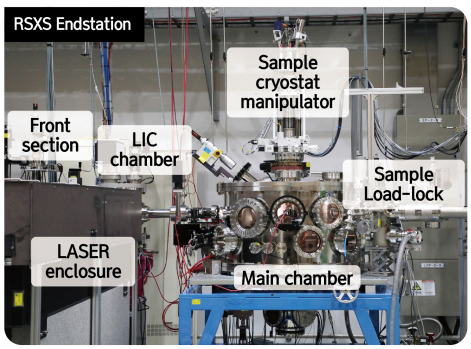
Insulator-to-Metal Transition Dynamics in Spatial Dependence at Femtosecond Timescales

A. S. Johnson *et al.*, *Nat. Phys.* **19**, 215 (2023)

Resonant Soft X-ray Scattering (RSXS) Endstation

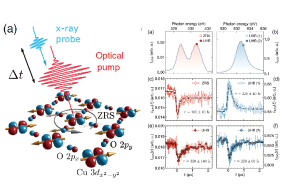
Experimental parameters

Laser incident angle	Collinear (<1°)
Laser wavelengths	240 nm ~ 2600 nm (800 nm harmonics, OPA)
Laser pulse duration	~40 fs (800 nm)
Sample motion	6-axis (3 rotations + 3 translations)
Sample temperature	Down to ~25 K (LHe) or ~90 K (LN_2)



Scientific cases

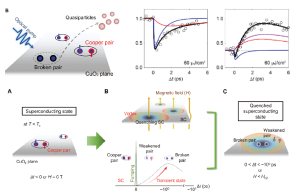
Light Engineering of Superconductor



Dynamic Hubbard U Renormalization in Superconductor Cuprate

D. R. Baykusheva, *et al.*, *Phys. Rev. X* **12**, 011013 (2022)

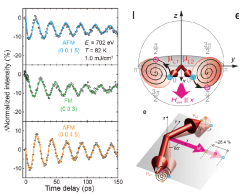
Realization of Out-of-Equilibrium States



From the Competition of Charge Order and Superconductivity in Cuprate

H. Jang, *et al.*, *Sci. Adv.* **8**, eabk0832 (2022)

4D Visualization of Coherent Magnon



Visualization of Ultrafast Magnetization of Optically Activated Coherent Magnon

H. Jang *et al.*, *Adv. Mater.* **35**, 2303032 (2023)

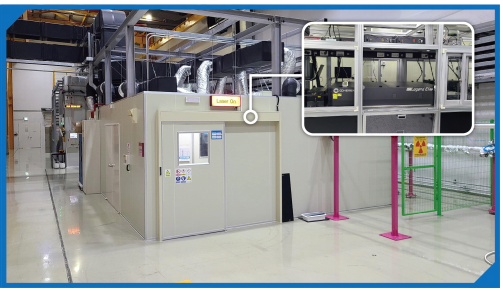
Optical Laser System

HX

Ti:sapphire Laser System	
Wavelength (nm)	~ 800
Rep. Rate (Hz)	< 120
Pulse Energy (mJ)	10 (max)
Pulse Width (fs, FWHM)	~ 40

Frequency Tuning System	
Harmonic Generator	400 nm, 266 nm
Optical Parametric Amplifier (OPA)	240 nm - 2600 nm
Optical Parametric Oscillator (OPO)	210 nm - 2600 nm (2 ~ 5 ns pulse width)

SX



Ti:sapphire Laser System	
Wavelength (nm)	~ 800
Rep. Rate (Hz)	< 720
Pulse Energy (mJ)	4 (max)
Pulse Width (fs, FWHM)	~ 40

Frequency Tuning System	
Harmonic Generator	400 nm, 266 nm
OPA	240 nm - 2600 nm

X-ray Detector

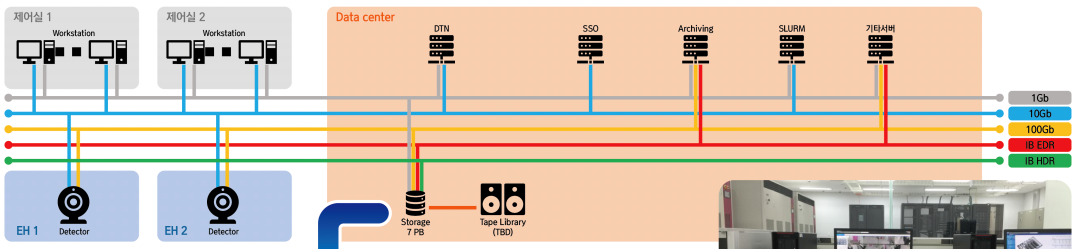
HX

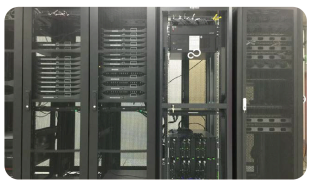
Detector	RAYONIX	JUNGFRAU
Pixel size (μm)	39 (MX) 44 (LX)	75
Pixel #	5760×5760 (MX) 5760×1920 (LX)	512×1024 / 0.5M
Area (mm²)	225×225 (MX) 255×85 (LX)	38×77 / 0.5M
Frame Rate (Hz)	10 (2×2 binning) 30 (4×4 binning) 60 (6×6 binning)	< 1.1 k
Op. Temp (℃)	-80	20

SX

Detector	ANDOR	PI-MTE	AXIS
Pixel size (μm)	13.5	13.5	6.5
Pixel #	2048×512	2048×2048	2048×2048
Area (mm²)	27.6×6.9	27.6×27.6	13.3×13.3
Frame Rate (Hz)	2.48	1.3 (4×4 binning)	35
Op. Temp (℃)	-85	-45	-20

Data System





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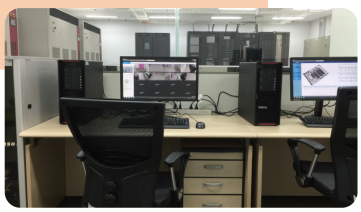

	Specification
Storage	7 PB @ 60 GB/s IO, Gen4
Network	IB HDR, IB EDR, 100 Gbps, 10 Gbps, 1 Gbps
Analysis Farm	R630, R730
Data Transfer Nodes	GSDC (KISTI) / PSC (POSTECH)