SACLA Users' Meeting 2022
March 2-3, 2022 (online)

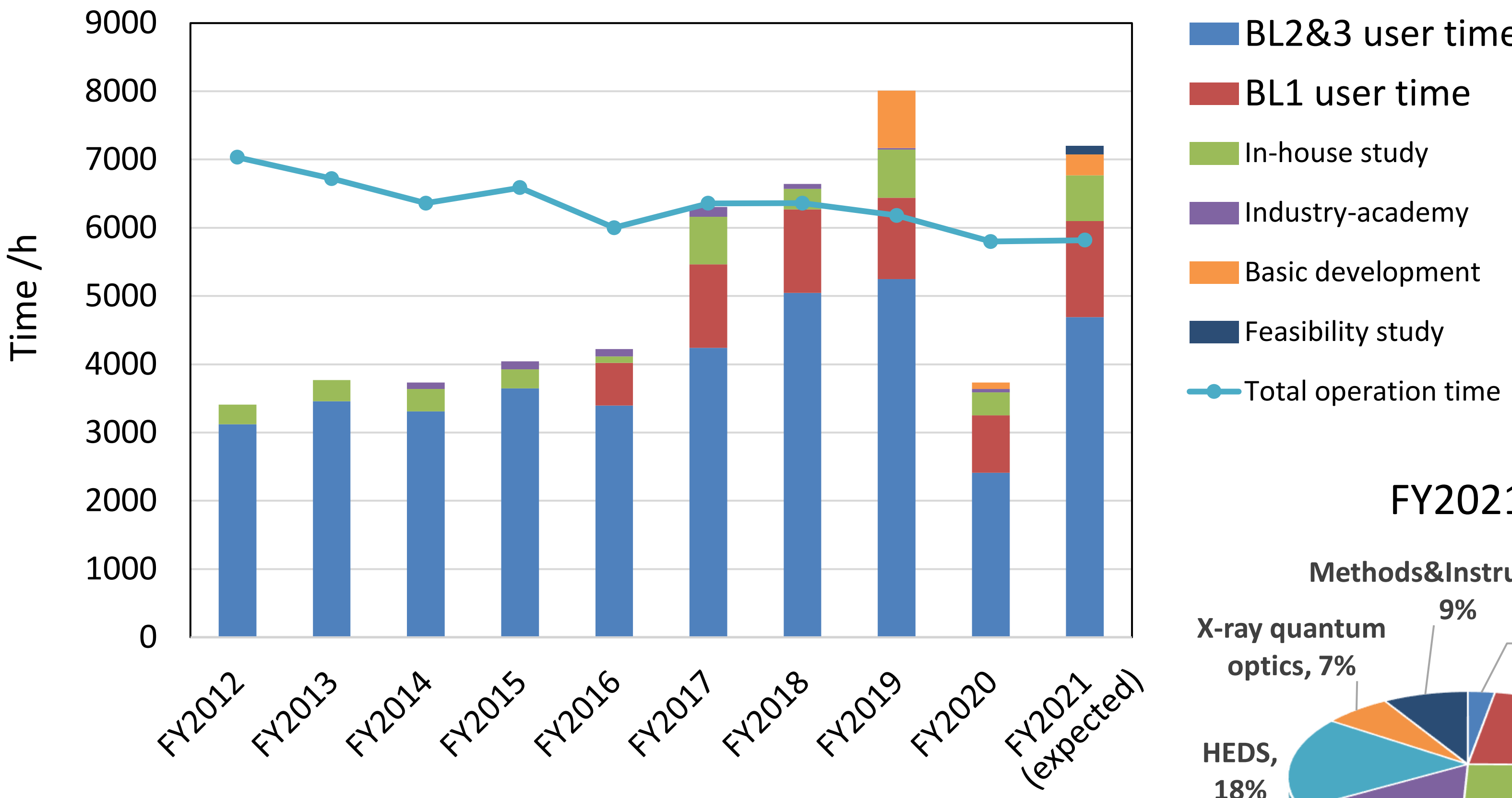
Facility update

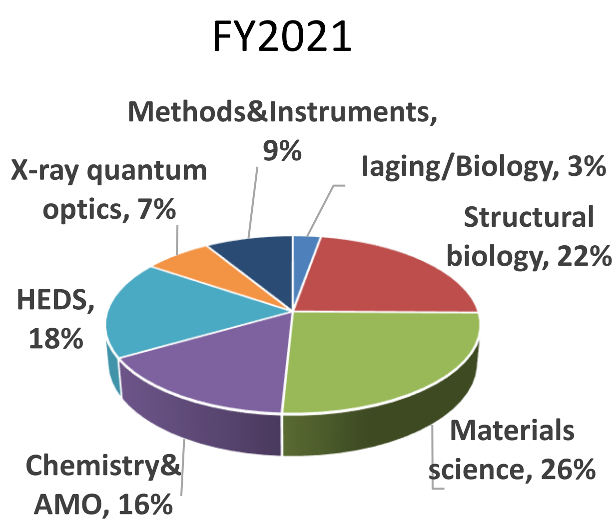
Kensuke Tono
on behalf of SACLA

Contents

- User operation
  - Beamtime & proposals in FY2021
  - Experiments under the COVID-19 pandemic
  - Research highlights
- Technical updates
  - Accelerator and beamlines
  - Experimental stations
- Summary

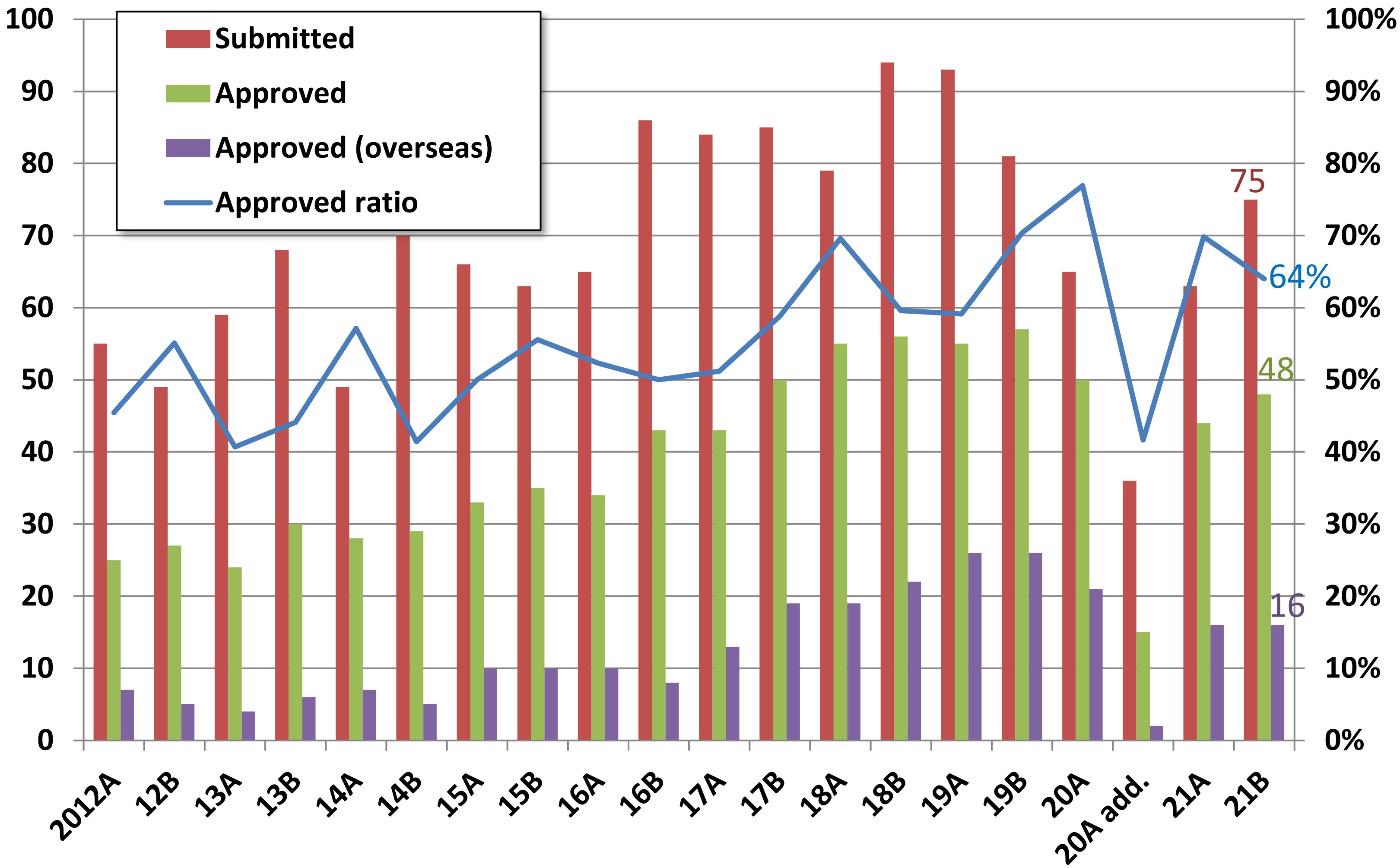
Operation time





- User time in FY2020 was about half the usual due to the COVID-19 pandemic.
- Will be at the same level as before in FY2021.

Number of proposals



- Number of proposals is recovering from the drop in FY2020.

User experiments in FY2021

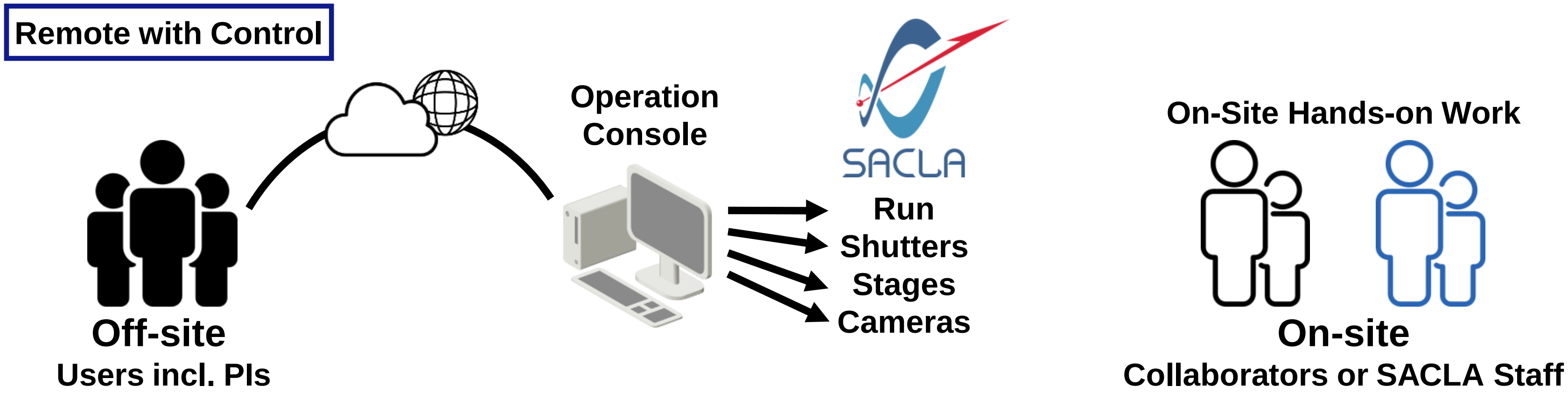
- Total beamtime in FY2021 will be on the same level as usual (~6,000 h).
- International users are still facing the strict travel restrictions.
- Only 5 cancellations in FY2021.
  - Domestic users: Mostly do experiments as before.
  - International users: Collaborators in Japan do hands-on works onsite.
- Some of the cancelled beamtimes were filled by proposals in a waiting list.
- Remote control system is now available for experiments using the high-power lasers (first pilot experiment in Feb 2022).

Number of projects (FY2021)

Term	Proposed	Approved	Cancelled	Additionally approved
2021A	63	44	1	1
2021B	75	48	4	2

Slide from the last meting (T. Yabuuchi)

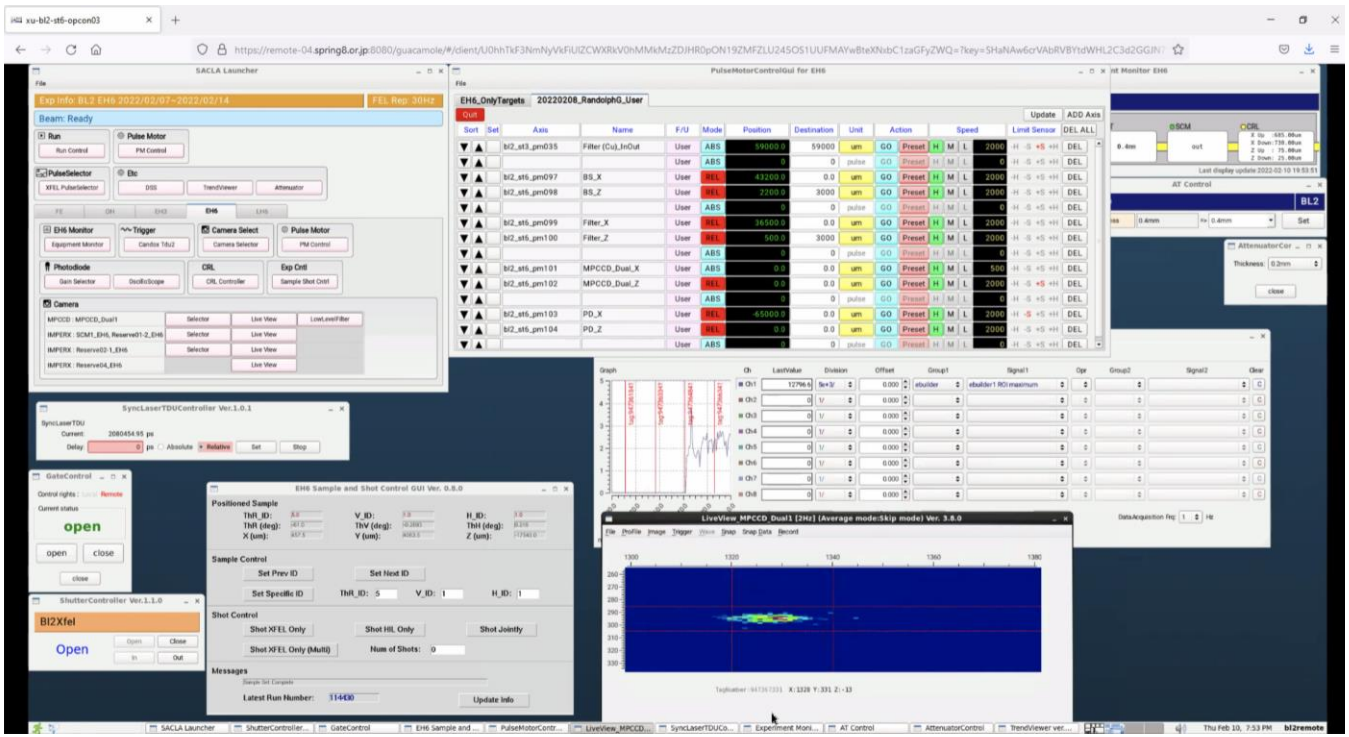
Conducting experiments remotely is beneficial to users and also the facility



- On-site participants can focus on hands-on work in the facility.
- Off-site participants can conduct routine processes for data acquisitions.
- A **hybrid style**, in which limited users visit SACLA and others joined remotely with control, can be also realized with the remote-control capability.
  - On-site users may not need to make 2-3 teams for the 24-hour operation, since the off-site team can take over a part of the shifts.
  - A few users may be enough just to prepare samples on-site or setup user-owned equipment, which are not done by the facility staff.

First remote experiments were performed at high-power laser platform

Users remotely operated beamline instruments and took >200 shots of high-power femtosecond laser with XFEL.



Remote access to the instruments and HPC system from European XFEL, HZDR (Germany) and Imperial College London (UK).

=> Cf: Breakout Session A2 (today)

SACLA Feasibility Study Program

- From 2021A
- Use SACLA on a trial basis for feasibility study.
- Available instruments:
  (1)DAPHNIS for serial femtosecond crystallography (SFX)
  (2)Experimental platform using the high-power nanosecond laser
- Maximum beamtime: 1 shift (12 hours).
- Co-application with the general SACLA Research Proposals is possible.

Term	Submitted	Conducted	
2021A	15	9	SFX: 3
			HP-nL[†]: 6
2021B	21	5	SFX: 3
			HP-nL[†]: 2

[†] Experiments using *high power nanosecond laser* & XFEL

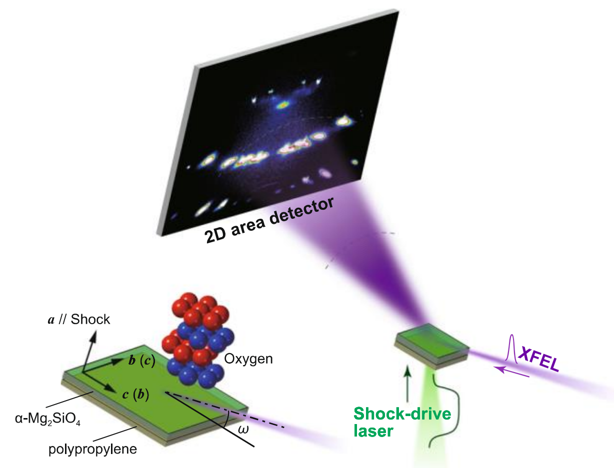
Research highlights (1)

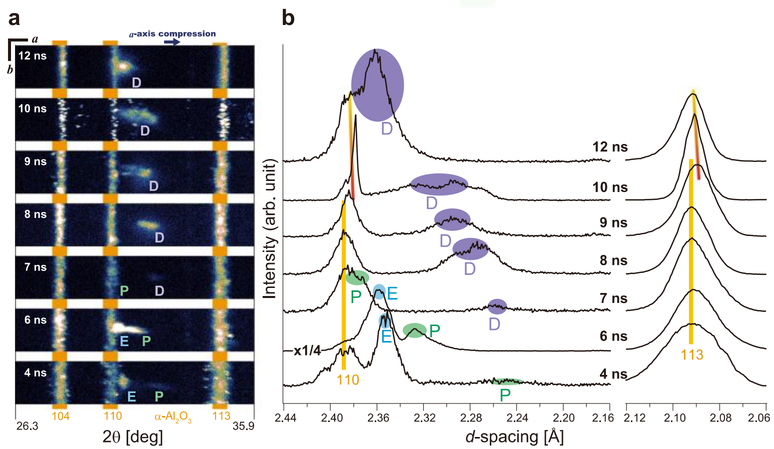
HED science

nature COMMUNICATIONS

Ultrafast olivine-ringwoodite transformation during shock compression

Okuchi et al., *Nat. Commun*. 12, 4305 (2021).





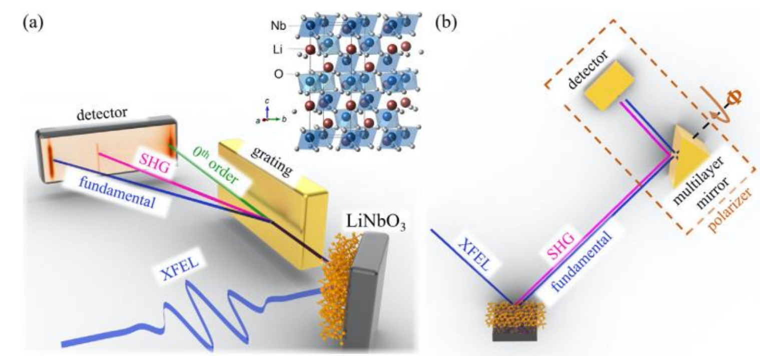
Nonlinear optics

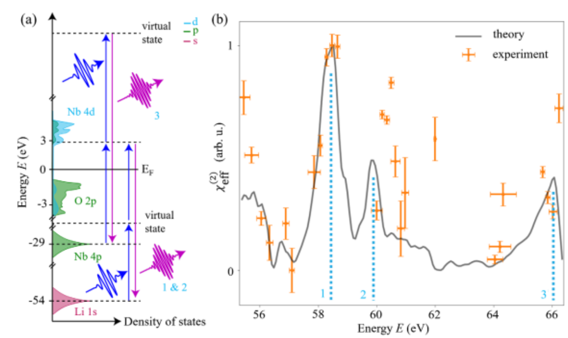
PHYSICAL REVIEW LETTERS **127,** 237402 (2021)

Polarization-Resolved Extreme-Ultraviolet Second-Harmonic Generation from $LiNbO_3$

Can B. Uzundal,[1,2] Sasawat Jamnuch,[3] Emma Berger,[1,2] Clarisse Woodahl,[1,4] Paul Manset,[5] Yasuyuki Hirata,[6] Toshihide Sumi,[7] Angelique Amado,[1,2] Hisazumi Akai,[7] Yuya Kubota,[8,9] Shigeki Owada,[8,9] Kensuke Tono,[8,9] Makina Yabashi,[8,9] John W. Freeland,[10] Craig P. Schwartz,[11] Walter S. Drisdell,[12,13] Iwao Matsuda,[14,7] Tod A. Pascal,[3,15,16,*] Alfred Zong,[1,2] and Michael Zuerch[1,2,17,18,†]

Uzundal, Zuerch *et al., Phys. Rev. Lett.* 127, 237402 (2021).





The instrument has been developed under SACLA Basic Development Program (Prof. Matsuda et al.)

=> Scientific Talk by Prof. Matsuda (today)

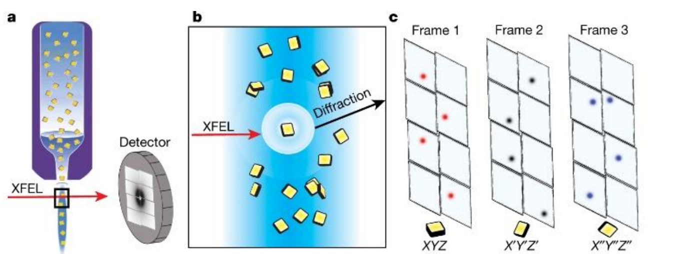
Research highlights (2)

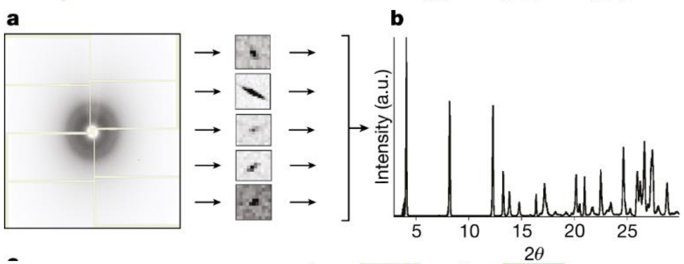
Materials science

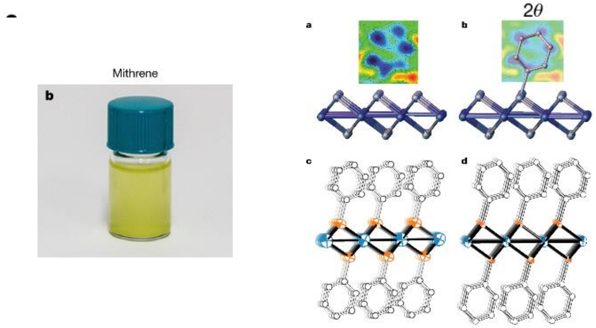
Small molecule serial femtosecond crystallography

Schriber, Hohman et al., *Nature* 601, 360 (2022).

Mithrene ($AgSeC_6H_5$), thiorene ($AgSC_6H_5$), tethrene ($AgTeC_6H_5$): Inorganic–organic hybrid materials



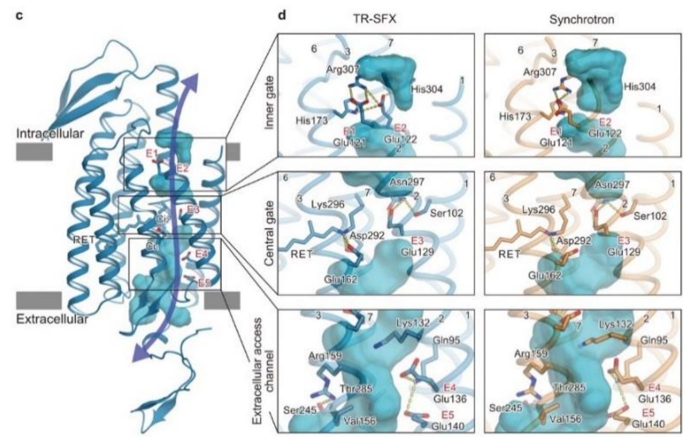


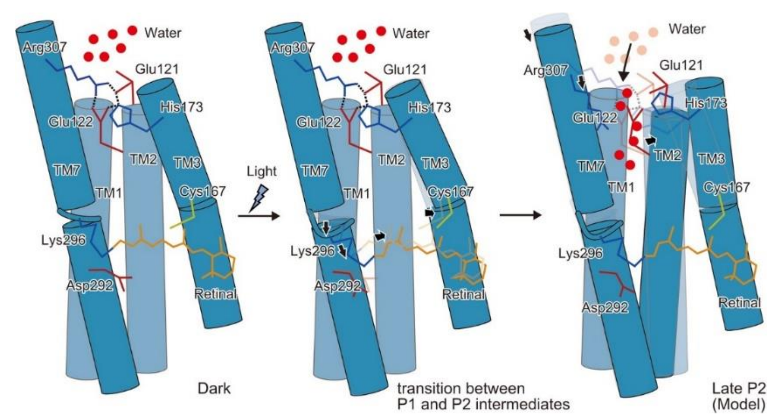


Structural biology

Time-resolved SFX to reveal early structural changes in channelrhodopsin

Oda, Nureki *et al., eLife,* 10:e62389 (2021).





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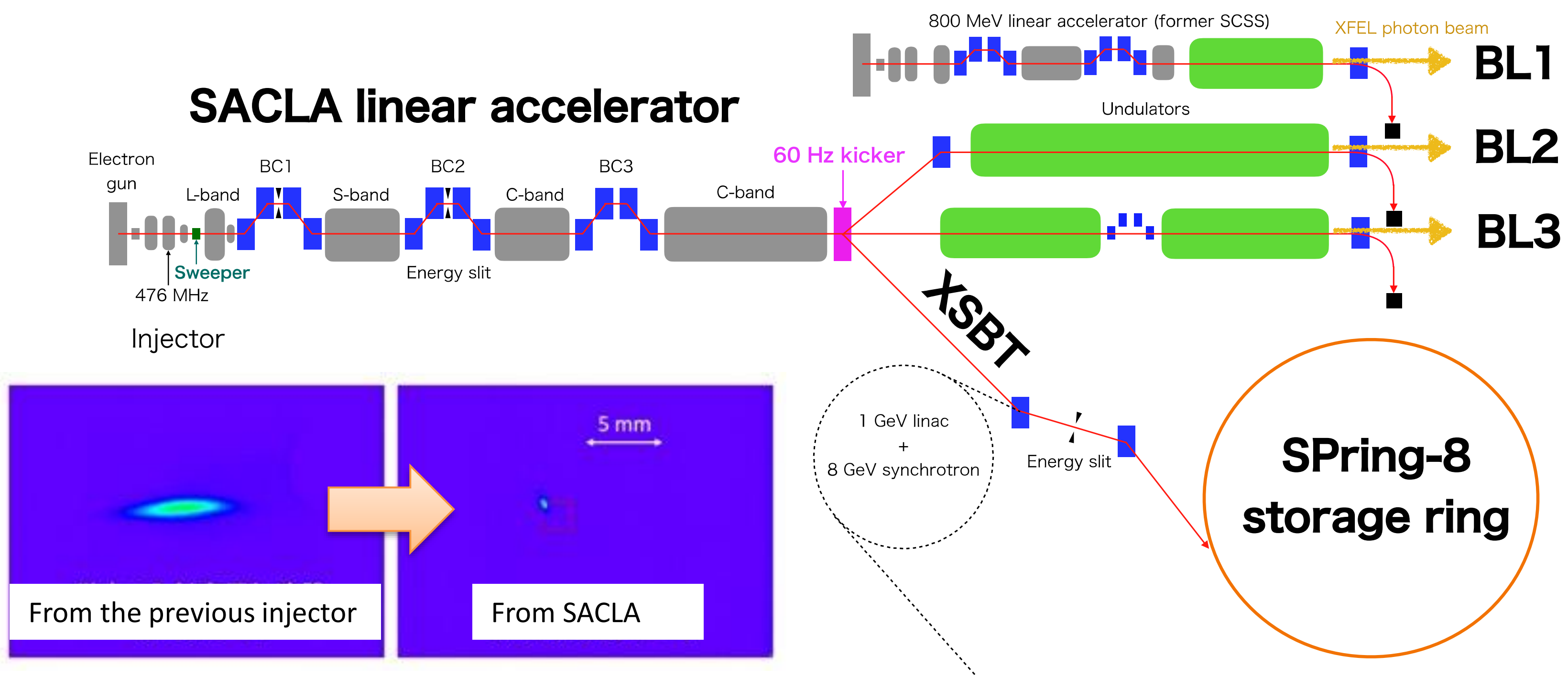
Electron beam injection to SPring-8

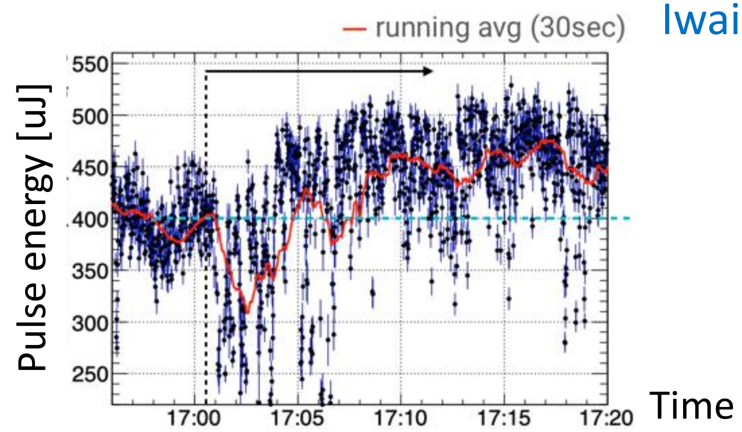
Hara et al., Phys. Rev. AB (2021)

- Full-time injection of higher-quality beam from SACLA to SPring-8.
- Important milestone for the SPring-8 upgrade project.
- Previous injector system was closed.
- Lower power operation for Green Facilities.



Automatic accelerator tuning based on machine learning

- To establish reliable tuning procedures without depending on the skills and experience of the operators.
- Auto-tuning system has already been used to maximize XFEL pulse energy in daily tuning.

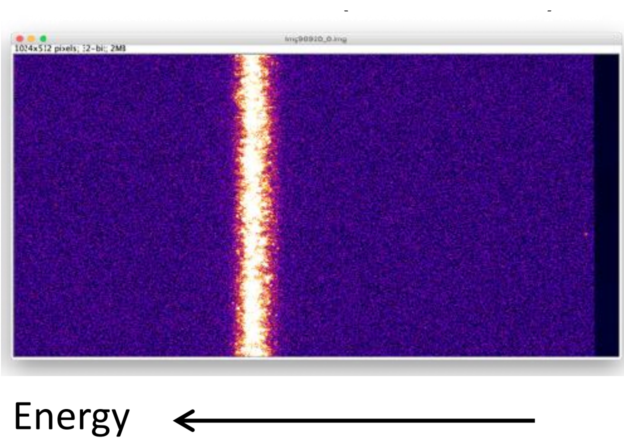


Iwai et al.

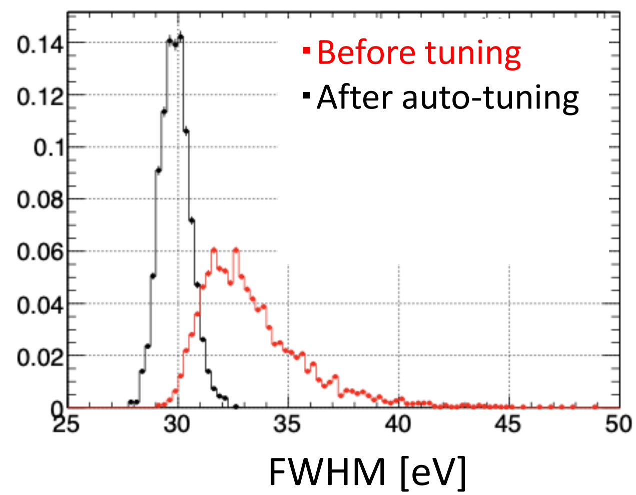
- *A new in-line spectrometer* allows the system to optimize a spectral shape.
  - Diamond powder in a capillary at a peripheral region of the XFEL beam.
  - Resolution is higher (a few eV) than existing one's (several-tens eV).

Inoue et al., J. Synchrotron Rad., in press.

Diffraction pattern on MPCCD



Frequency distribution of spectral FWHM

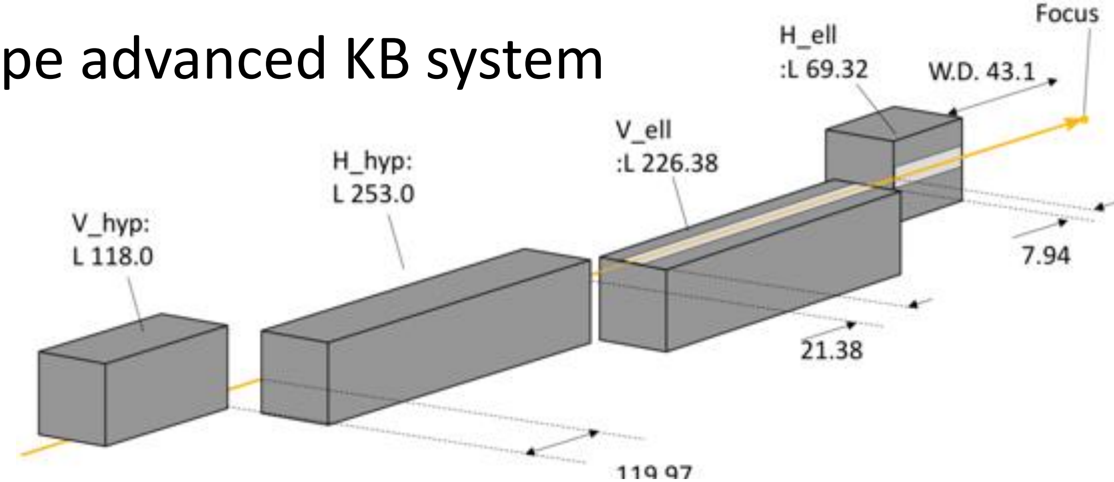


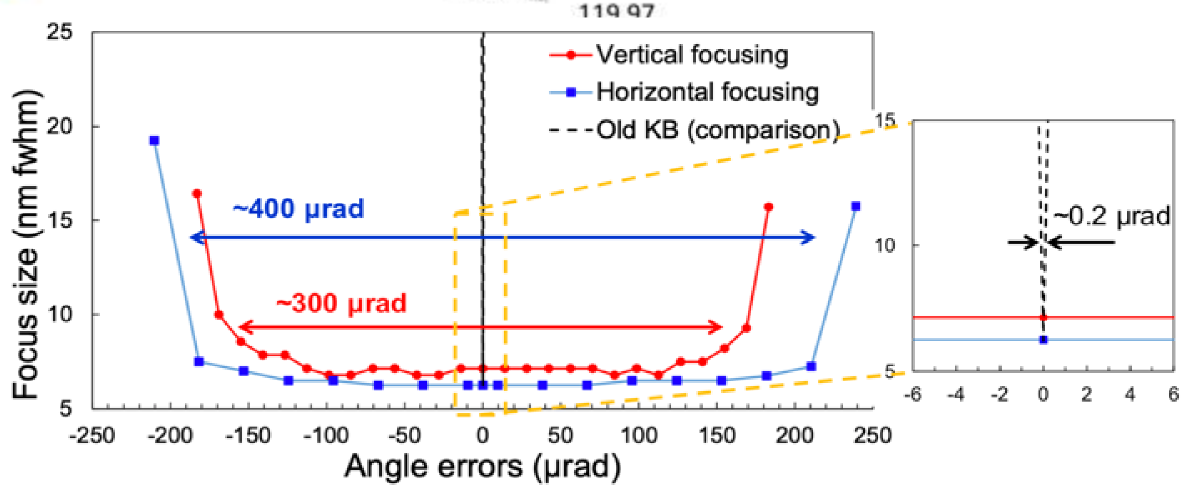
Sub-10 nm focusing system at BL3

Basic Development Program (Prof. Yamauchi et al.)
=> Report tomorrow

Wolter-III type advanced KB system

Yamada et al.





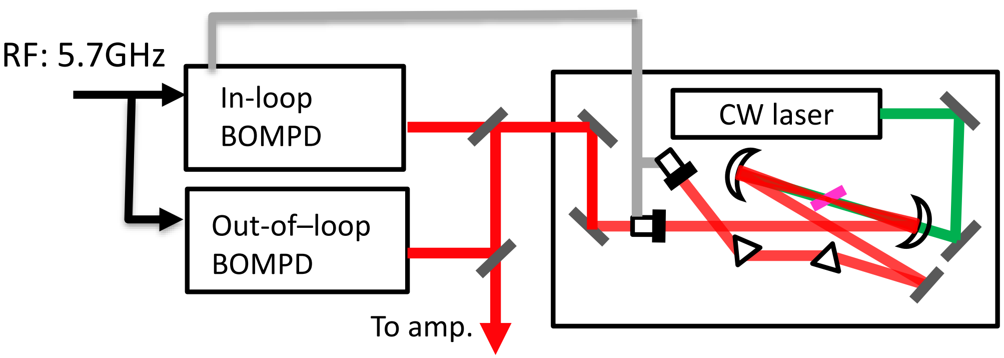
Large angular-error tolerance: 300-400 μrad.

(~1,000 times as large as conventional KB)

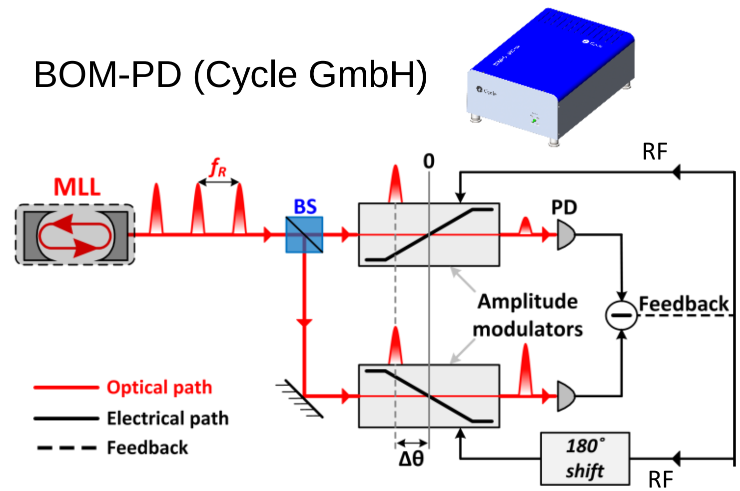
Synchronized fs laser system: Improved timing synchronization with XFEL

Togashi et al.

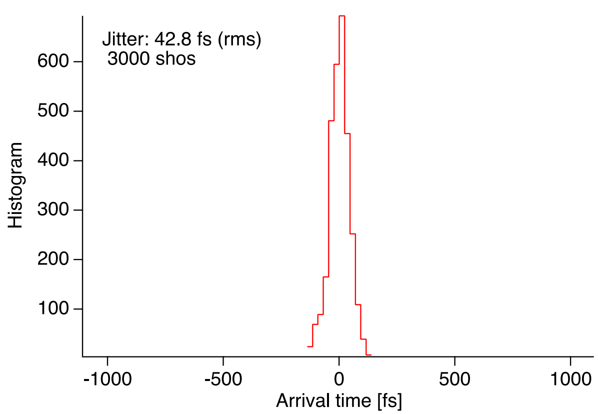
Synchronization using BOM-PD



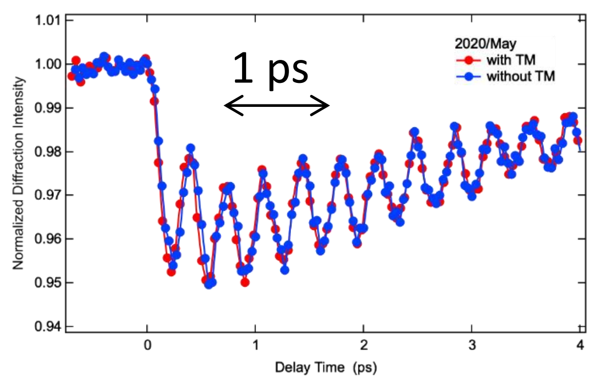
BOM-PD (Cycle GmbH)



Jitter: ~40 fs (rms, 5 minutes)
Drift: ~±0.5 ps (24 hours)



Time-resolved XRD of Bi



A feedback system is under development to suppress the long-term drift of the laser timing.

SACLA/SPring-8 Basic Development Program

Progress reports of Projects 1-6 will be given tomorrow.

FY2021: 13 proposals were approved.

Seven proposals for full approval to proceed with instrument developments

1. Development of multispectral imaging system by aperture division of *rotational soft X-ray mirror* (PI : T. Kimura, U. Tokyo)
2. X-ray experiment in *pulsed ultrahigh magnetic field* beyond 100 T with a portable single turn coil system "PINK" (PI : A. Ikeda, UEC Tokyo)
3. Measurement systems for *biomolecular movies* using X-ray free electron lasers (PI: S. Iwata, Kyoto U.)
4. Time Resolved *Resonant Inelastic X-Ray Scattering* Beyond Iridium (PI : M. P. M. Dean, BNL)
5. Development of a wide-dynamic-range and high-frame-rate *CMOS image sensor for soft X-ray* II (PI : T. Arima, U. Tokyo)
6. Development of *sub-10 nm XFEL focusing system* based on novel imaging mirror optics (PI: K. Yamauchi, Osaka U.)
7. Development of pair distribution function measurement of liquids and amorphous materials under high pressure and high temperature conditions (PI : Y. Kono, Ehime U.) (SPring-8)

Six proposals for partial approval (feasibility studies are required)

Instruments available soon:

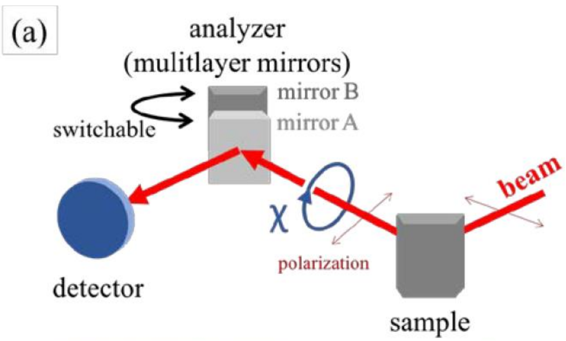
- Experimental system for SX-FEL opto-spintronics (Prof. Matsuda et al.)
- Sub-10 nm XFEL focusing system (Prof. Yamauchi et al.)

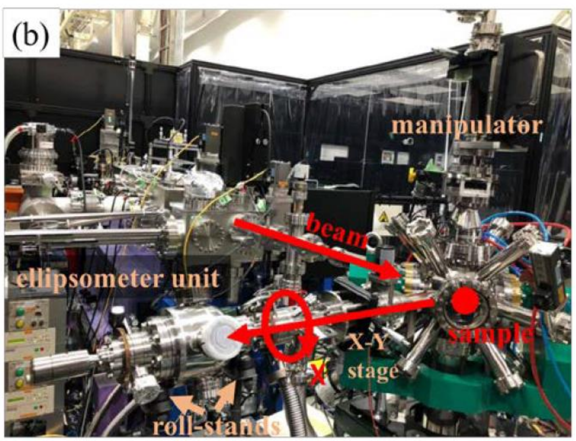
Experimental system for SX-FEL opto-spintronics

SACLA Basic Development Program (Prof. Matsuda, Prof. Mimura et al.)

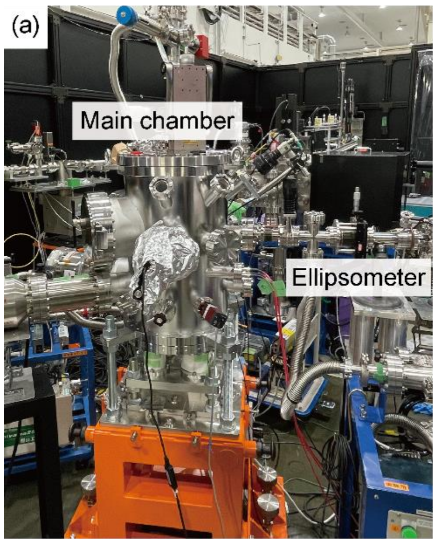
Araki, Matsuda et al., e-J. Surf. Sci. Nanotechnol. (2020).
Sumi, Horio, Matsuda et al., e-J. Surf. Sci. Nanotechnol. (2022).

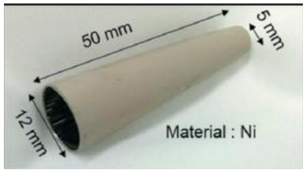
Type I

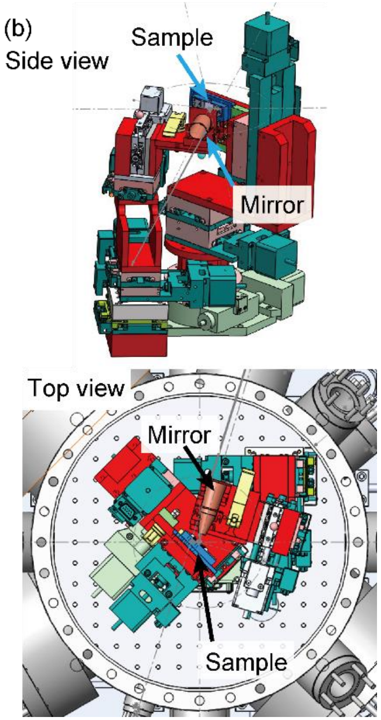




Type II







Pilot experiments in 2021B

=> Scientific Talk by Prof. Matsuda (today)

XFEL experimental system with high-power nanosecond laser

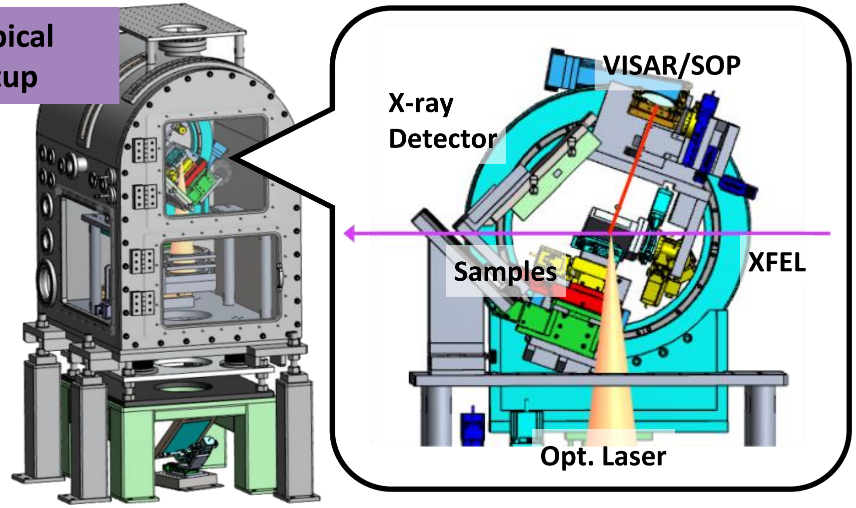
Experimental platform specifically developed for laser-shock experiments

Hutch		EH5 at BL3
Optical Laser	Max. Energy (typ.)	~15 J
	Pulse Duration (typ.)	5 ns
	Wavelength	532 nm
	Rep. Rate	0.1 Hz
XFEL	Focus with KB Mirrors	>0.5 µm

OSAKA UNIVERSITY

High-energy optical laser has been installed in collaboration with Osaka University.

Typical Setup

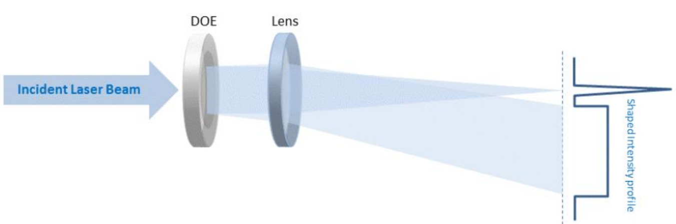


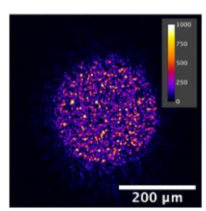
Inubushi et al., Appl. Sci. 10, 2224 (2020)

Recent upgrade

SACLA Basic Development Program (Prof. Ozaki et al.)

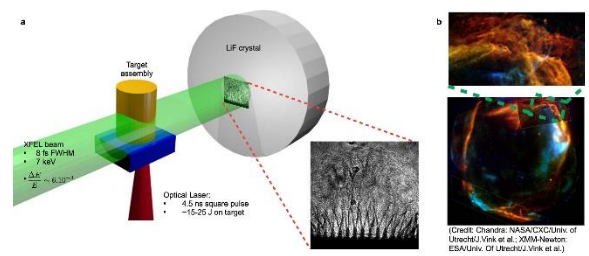
Diffractive optical elements (DOEs) for focal spot smoothing



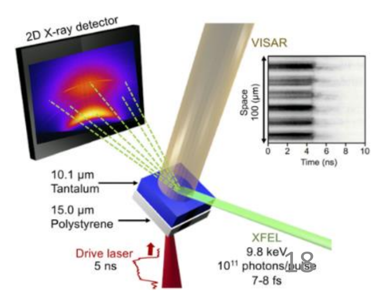


Recent Remarks

G. Rigon, M. Koenig et al., "Micron-scale phenomena observed in a turbulent laser-produced plasma", Nat. Commun. ***12****, 2679 (2021).*



K. Katagiri, N. Ozaki et al., "Micron-scale phenomena observed in a turbulent laser-produced plasma," Phys. Rev. Lett. 126, 175503 (2021).



=> Scientific Talk by Prof. Ozaki (today)

CITIUS Detector: XFEL variants

Architecture [1-3]

Integration Pixel & High Frame Rate

Feature

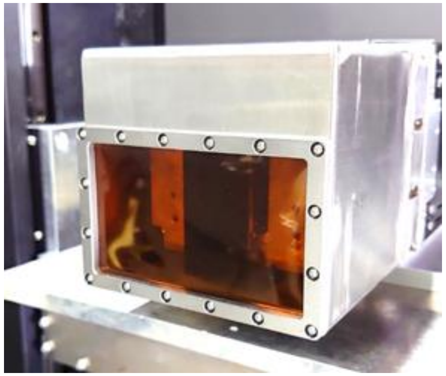
Zero Noise	Spectro-Imaging	High Spatial Resolution	High Dynamic Range	Ultralow Systematic Error

Confirmed Performance at the Component level

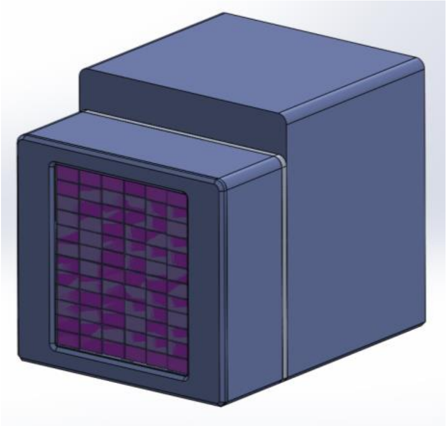
Parameters		Value
Sensor	Photodiode thickness	650 µm
	Pixel Size	72.6 µm
	Noise	0.02 phs.@12 keV
	Peak Signal	9,000-10,000 phs.@12 keV
	Frame Rate	60 Hz (max. 5 kHz)
	Pixel Number	0.28 Mpixel/sensor
Largest System	Pixel Number	20.2 Mpixel
	Image Area	322 x 364 mm^2

Schedule

2013: Project started
2015: Partners agreed
2020 Sep: First light of one modular system in final form
2021 Dec: Start of the assembly of 20.2M pixel system
2022: In-kind user operation



First detector under evaluation



20.2 Mpixel system for SACLA

1) SPring-8 II CDR (2014) with updated values.
2) T. Hatsui, presented at iWorld (June. 2014).
3) T. Hatsui, AOSFRR (Nov. 2015)

SACLA HPC - System was updated in Sep., 2021

Main Changes;

- Introduced Environment Modules.

- see: http://xhpcfep.hpc.spring8.or.jp/document/about_environment_modules.html

- Changed the PBS queue settings.

- see: http://xhpcfep.hpc.spring8.or.jp/document/queue_configuration.html

- The SACLA analysis software was updated.

- see: http://xhpcfep.hpc.spring8.or.jp/release/2021-09-01-01-offline001.html

Contact for technical inquiries: SACLA HPC HelpDesk (hpc-helpdesk@spring8.or.jp)

Posters from the facility

Please find poster files on the on-line program:
http://xfel.riken.jp/usersmeeting2022/program.html

1. Overview of SACLA Beamlines (BL1, 2, 3) (T. Osaka, Y. Inubushi)
2. Standard Instrument for Serial Femtosecond Crystallography (SFX) (Tono, Owada, Joti)
3. Standard Instruments for X-ray Diffraction and Scattering (Kubota, Osaka, Togashi, Owada)
4. Capabilities of Intense X-ray Sciences at BL3 (Inoue, Yamada, Osaka, Inubushi)
5. Synchronized Optical Laser System at SACLA (Togashi, Owada)
6. Experimental Platform for High-power Nanosecond Laser with XFEL at SACLA (Miyanishi, Sueda, Inubushi, Yabuuchi)
7. Experimental Platform with High-power Femtosecond Laser at SACLA (Yabuuchi, Sueda, Inubushi, Miyanishi, Togashi, Tomizawa)
8. Diffraction-limited Resolution Scintillator Detector (Kameshima, Hatsui)
9. Progress Report on "Experimental Support and Information Sharing" after SACLA Users' Meeting 2021 (Language: Japanese)

Summary

- 10 years since the start of user operation.
- SACLA operation is returning to normal after the impact of the pandemic.
  - Domestic users have access to SACLA and do experiments as usual in FY2021.
  - Most international users remotely participate in their experiments, where collaborators in Japan do hands-on work onsite.
  - Only 5 projects were cancelled in FY2021.
  - Remote-with-control system has started operation.
- SACLA has been technically upgraded for the next 10 years with:
  - Beam injection to SPring-8,
  - Automatic operations,
  - Remote experimentation,
  - Advanced beamline optics, photon diagnostic systems, and experimental instruments.

We would like your input.

Thank you for your support for 10 successful years.

http://xfel.riken.jp/index.html