SACLA Users' Meeting 2024

Update of Standard System for Serial Femtosecond Crystallography at SACLA

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Major updates

- Femtosecond laser is available at BL2 EH3 from 2024A. ➡ ***Poster #1 & #2***
- A belt conveyor setup has been developed for serial femtosecond crystallography (SFX). ➡ ***Breakout session B***
- CITIUS 20.2M is under development for SFX at SACLA. ➡ ***Poster #3 & #4***

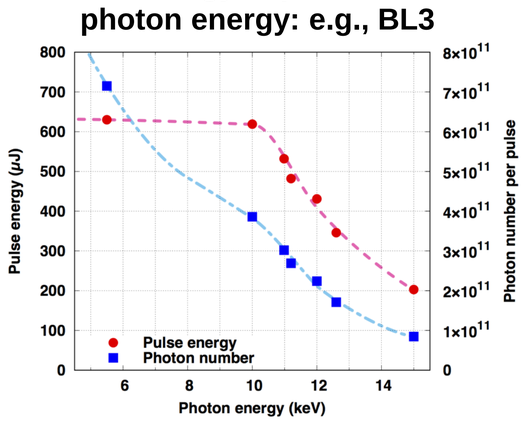
XFEL condition

Specifications of beamlines 2 and 3

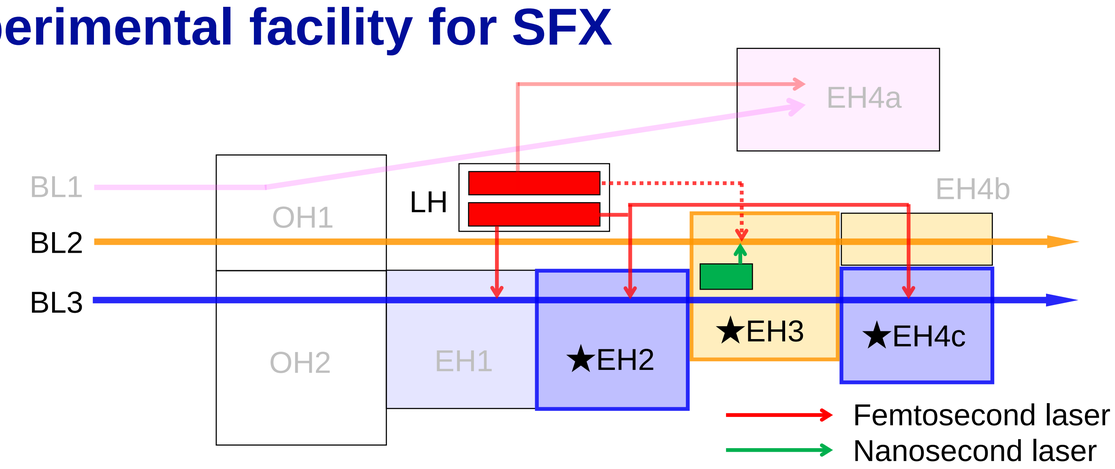
Photon energy	4 – 22 keV
Pulse width	< 10 fs (FWHM, fixed)
Repetition	30 / 60 Hz
Pulse energy (Pink beam)	BL2: ~500 µJ @10 keV BL3: ~700 µJ @10 keV (up to 900 µJ)
Beam size	EH3 & EH4c: ~1 µm FWHM EH2: >2 µm FWHM

(See ***Poster* #1** for detailed information).

Pulse energy dependence on photon energy: e.g., BL3



Experimental facility for SFX



Pump-probe measurement using lasers

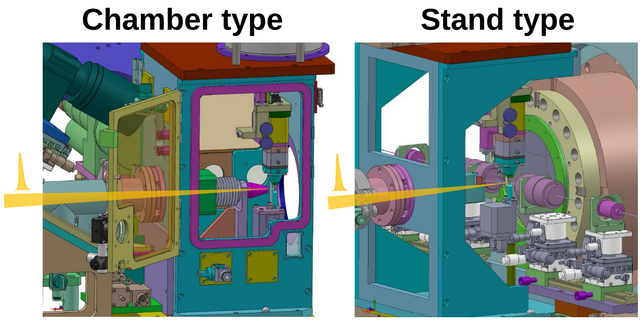
- Nanosecond or femtosecond laser pulses excite samples (pump).
- XFEL pulses are used to take diffraction patterns of the samples at transient states (probe).
- Wide delay time ranges from femtoseconds to milliseconds (or longer).
- Available femtosecond laser pulses at BL2 EH3 from 2024A.

See ***Poster* #1 & #2** for detailed information.

	Ti:sapphire with OPA	Nd:YAG	OPO
Wavelength	250 - 2600 nm	532 nm	210 - 2600 nm
Pulse duration	~40 fs (800 nm), ~70 fs (VIS/NIR)	~5 ns	~5 ns
Repetition rate	≤ 60 Hz	≤ 15 Hz	≤ 30 Hz
Pulse energy	~10 mJ (800 nm)	< 10 mJ < 30 µJ[1)]	< 1 mJ < 30 µJ[1)]
Typical spot size at sample	~150 µm (FWHM, Gaussian)	~80 µm[2)] (FWHM, Gaussian[3)]) 40 - 250 µm[4)] (through an optical fiber)	~150 µm[2)] (FWHM, Gaussian[3)]) 40 - 250 µm[4)] (through an optical fiber)
Experimental hutch	BL3 EH2, EH4c BL2 EH3[5)]	BL2 EH3	BL2 EH3
Remark	[1)] For the optical-fiber option. [2)] Using plano-convex lens [3)] Optional: Top-hat beam profile [4)] Dependent on the fiber core size [5)] Available from the season 2024A (➡ *Poster #2*)		

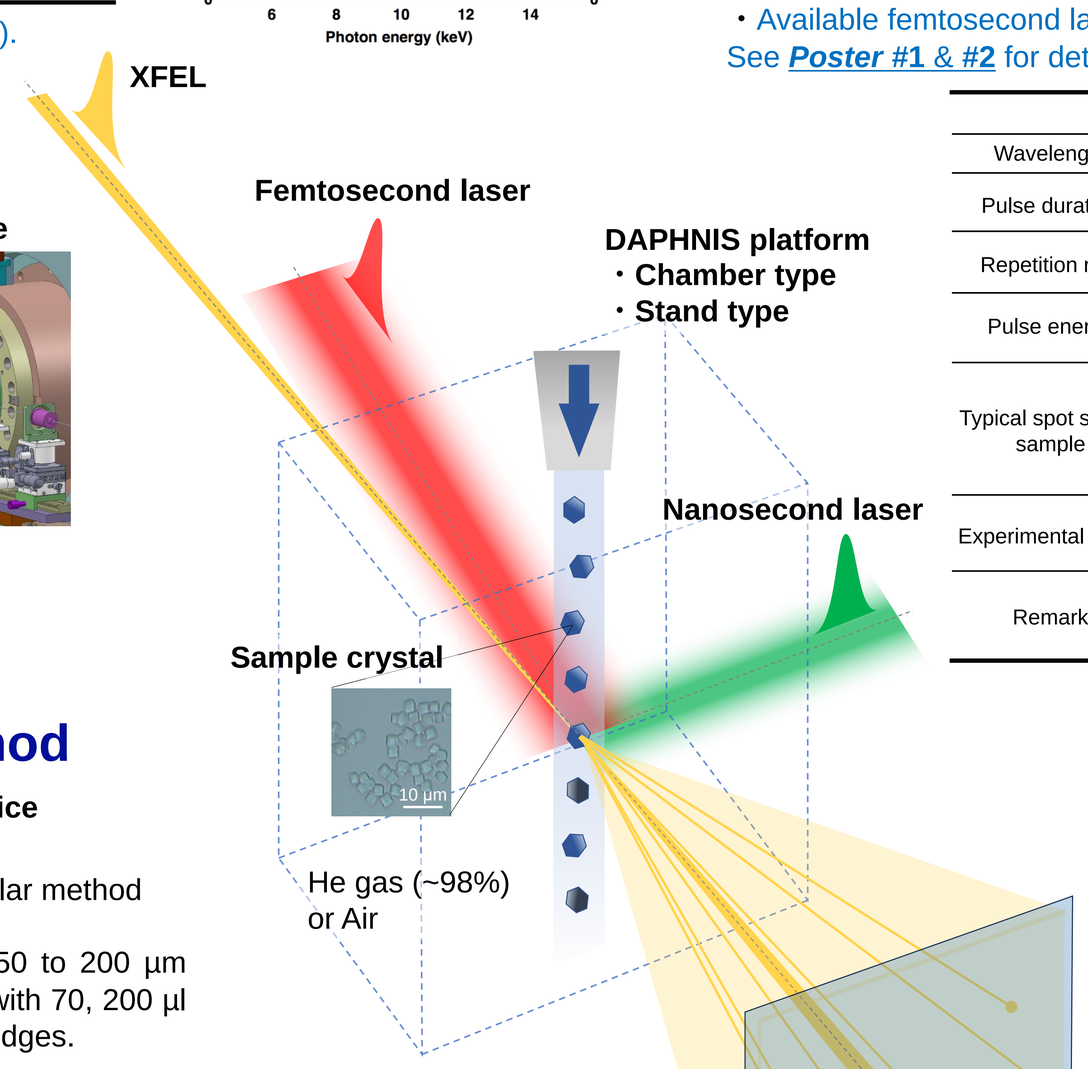
DAPHNIS platform

Chamber type **Stand type**



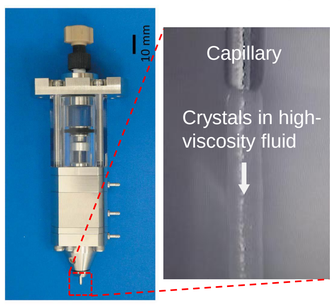
- Filled with Helium gas
- Air exposure

K. Tono et al., *J. Synchrotron Rad.* **22**, 532 (2015).
M. Kubo et al., *J. Synchrotron Rad.* **24**, 1086 (2017).



Sample delivery method

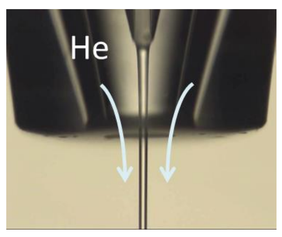
High-viscosity sample injection device



- Most popular method at SACLA.
- Available 50 to 200 µm capillary ID with 70, 200 µl sample cartridges.
- Available for pump-probe time-resolved SFX.

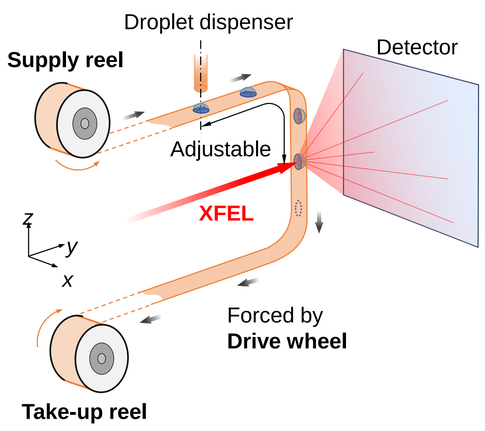
Y. Shimazu et al., *J. Appl. Cryst.* **52**, 1280 (2019).

Liquid-jet injector with a gas dynamic virtual nozzle (GDVN)

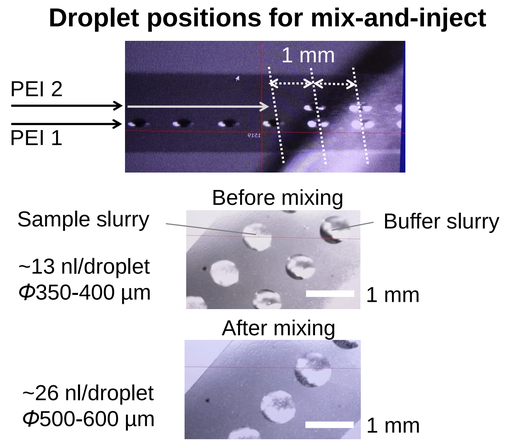


- Generally popular method, especially for mix-and-inject time-resolved SFX.
- Available ID of 50 to 200 µm inner capillary.
- Delay time ranges from 10 ms to seconds (or longer) for mix-and-inject time-resolved SFX.
- On development for reducing sample consumption.

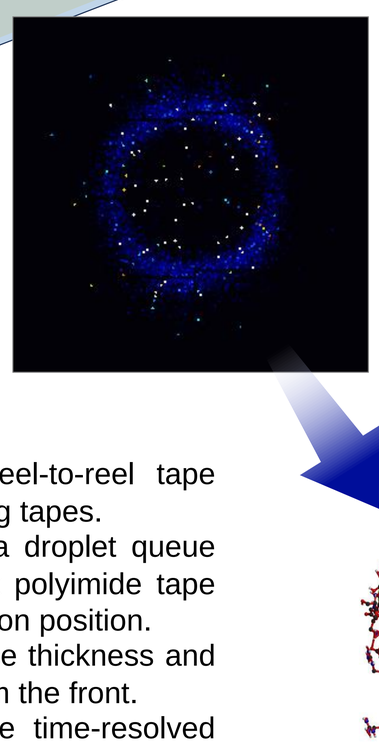
Belt conveyor setup (release to users in FY2024: Join ***Breakout session B*** for detailed information)



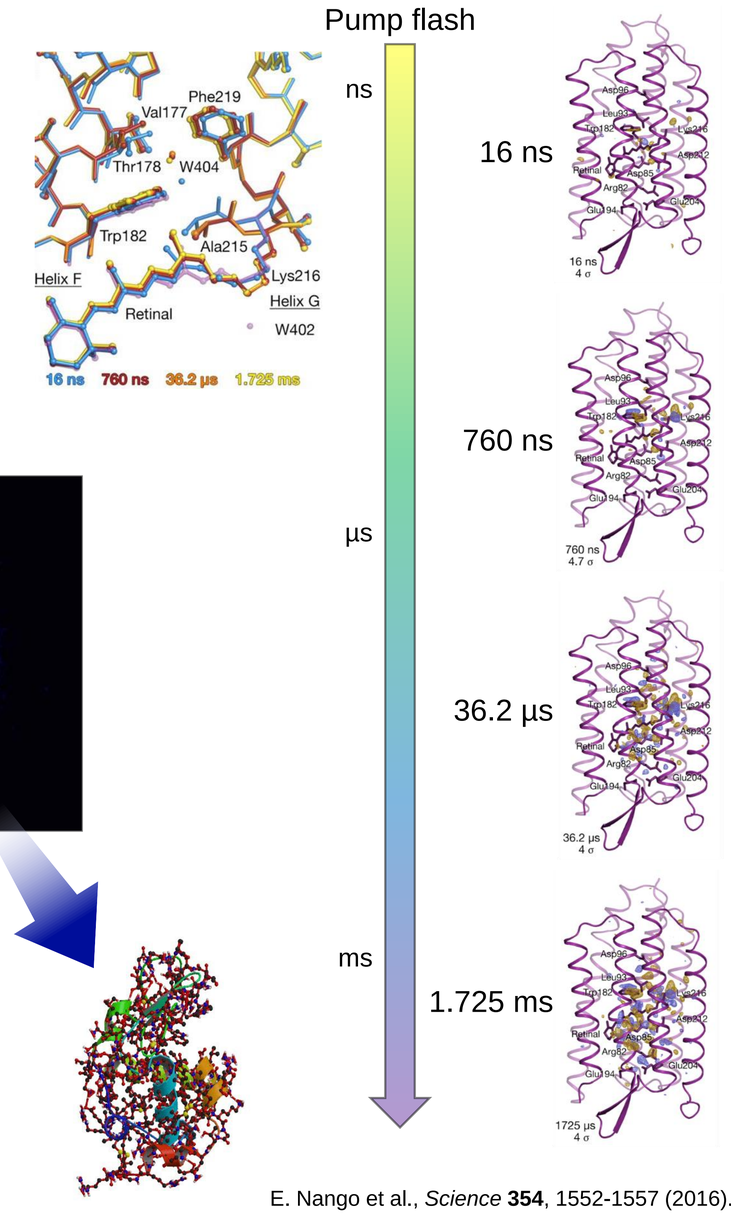
Droplet positions for mix-and-inject



- Designed as a compact reel-to-reel tape conveyor setup without recycling tapes.
- Dispense sample slurry as a droplet queue by the PEI onto 12.5 µm-thick polyimide tape and deliver to the XFEL irradiation position.
- XFEL pulses transmit the tape thickness and irradiate the sample droplet from the front.
- Mix-and-inject & pump-probe time-resolved SFX is under development.



Applications: Taking a molecular movie of bacteriorhodopsin



E. Nango et al., *Science* **354**, 1552-1557 (2016).

Standard detector

- MPCCD SWD is the most popularly provided detector for SFX at SACLA.

T. Kameshima et al., *Rev. Sci. Instrum.* **85**, 033110 (2014).

- CITIUS 20.2M is under development for SFX at SACLA as the largest direct X-ray detector in the world.

(See ***Poster* #3 & #4** for detailed information)

Specifications of the detectors for SFX at SACLA

	4M-pixel MPCCD (phase III SWD type)	Rayonix MX300-HS	**CITIUS 20.2M (under development)**
Frame rate	60 fps	10 fps @ 2x2 Binning 30 fps @ 4x4 Binning	60 fps
Standard camera distance in DAPHNIS platform	50 mm	75 mm or longer @Open stand	n/a
Active area	100 mm x 100 mm	300 mm x 300 mm	W321 mm x H393 mm
Achievable resolution on the detector edge	~0.15 nm @10 keV	~0.11 nm @10 keV, 4x4 Binning	n/a