Standard Instrument for Serial Femtosecond Crystallography (SFX)

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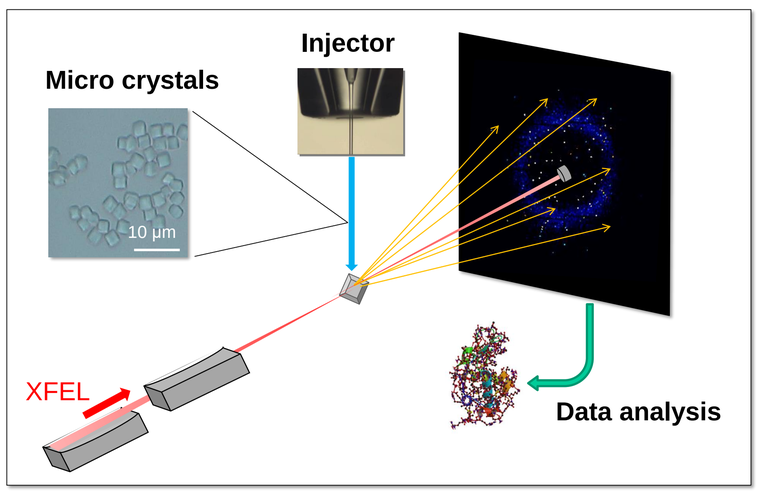
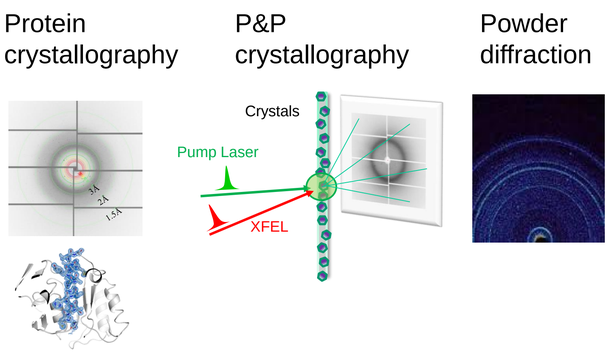
Serial femtosecond crystallography (SFX) is a method which allows users to analyze radiation-damage-free structures of micrometer- or sub-micrometer-scale crystals at room temperature. This method has a high compatibility with pump & probe measurement for studying fast dynamics. SACLA offers users an experimental platform for SFX, Diverse Application Platform for Hard X-ray Diffraction in SACLA (DAPHNIS). Users can select a variety of sample injectors according to their samples. This instrument is capable of pump & probe measurement with nanosecond or femtosecond optical lasers.

Diverse Application Platform for Hard X-ray diffraction in SACLA (DAPHNIS)

SFX

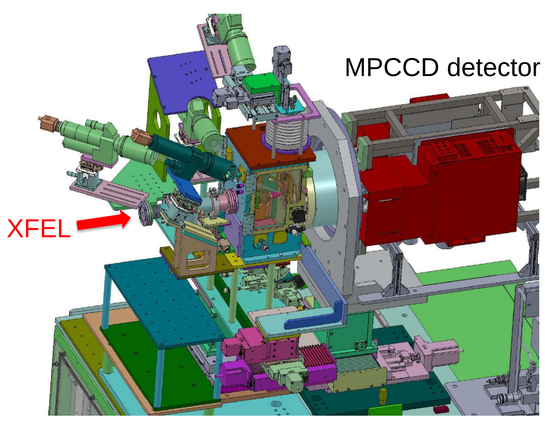


Applications



Parameter/device for DAPHNIS	Value/option	Remark
Standard detector	4M-pixel MPCCD[1)] (Phase III type)	Rayonix MX300-HS (10 Hz) is also available.
Frame rate	30 fps	
Standard camera distance	50 mm	
Active area of the detector	110 mm x 110 mm	8 sensor panels
Achievable resolution	0.15 nm at 10 keV	On the detector edge
Injector	High-viscosity sample-injection device[2)]	
	Liquid-jet injector	
	Droplet injector[3)]	
Typical hit rate	20-30%	
Typical index rate	60-70% of hit images	
Typical number of images to obtain a complete dataset (molecular replacement)	~1x10^4	For static structures
	~2x10^4	For pump & probe measurement
Optical laser for pump & probe measurement	fs OPA (BL3 EH2)	Wavelength tunable
	ns Nd:YAG (BL2 EH3)	λ = 532 nm
	ns OPO (BL2 EH3)	Wavelength tunable

DAPHNIS

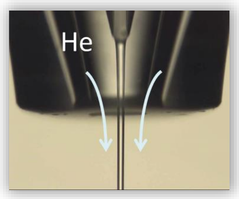


K. Tono et al., J. Synchrotron Rad. **22**, 532 (2015).
M. Kubo et al., J. Synchrotron Rad. **24**, 1086 (2017).

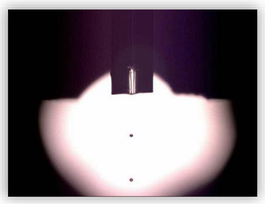
Sample injectors

High-viscosity sample-injection device

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



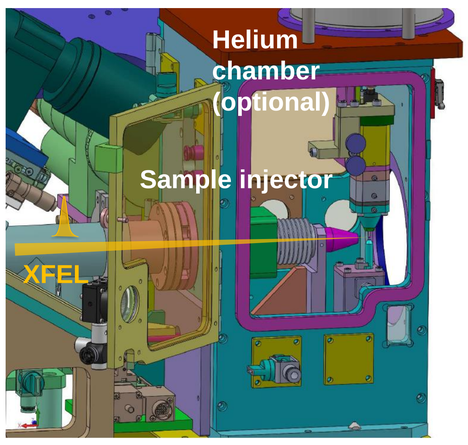
Droplet injector



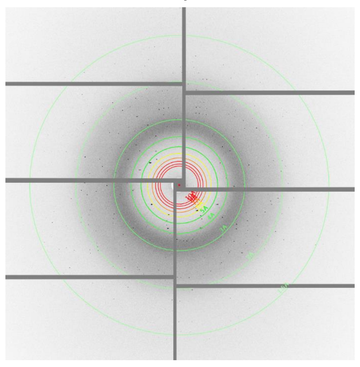
[1)] T. Kameshima et al., Rev. Sci. Instrum. **85**, 033110 (2014);.
[2)] Y. Shimazu et al., J. Appl. Cryst. **52**, 1280 (2019).
[3)] F. Mafuné et al., Acta Cryst. D**72**, 520 (2016).

Damage-free structure analysis

- Precise structures of micrometer or sub-micrometer crystals.
- Applicable even to crystals that are vulnerable to radiation damage.
- Major application: Protein crystals at room temperature.



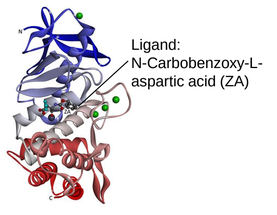
Diffraction pattern



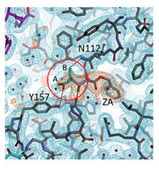
Application

Protein-ligand complexes being close to physiological conditions

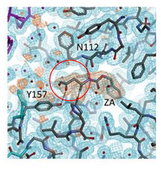
Thermolysin-ligand complex



Room temperature (XFEL)



Cryogenic condition (synchrotron radiation)

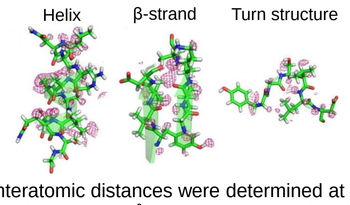


H. Naitow et al., Acta Cryst. D**73**, 702 (2017).

High-resolution analysis at room temperature

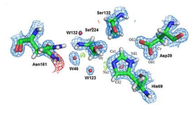
Proteinase K (partial structures)

Helix β-strand Turn structure



Interatomic distances were determined at a resolution of 1.2 Å. Hydrogen atoms (marked in red) are distinguishable.

Structure around the active site



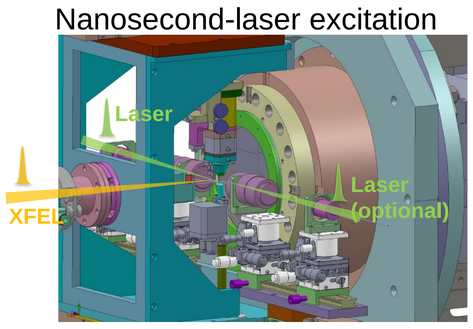
Water molecules (W46, W123, W132) are discernible.

T. Masuda et al., Sci. Rep. **7**, 45604 (2017).

Pump & probe measurement

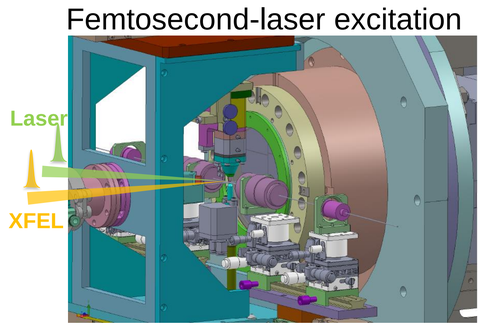
- Nanosecond or femtosecond laser pulses excite samples (pump).
- XFEL pulses are used to take diffraction patterns of the samples at transient states (probe).
- Wide delay-time range from femtoseconds to milliseconds (or longer).

Nanosecond-laser excitation



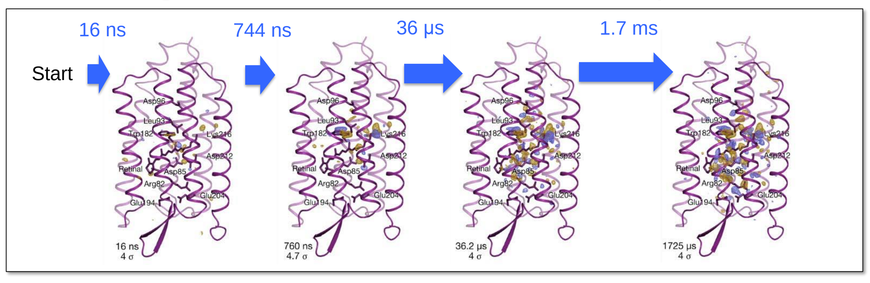
Double-side excitation is possible using optical fibers (optional)

Femtosecond-laser excitation



Near collinear excitation.
Timing monitor available (BL3).

Application: Taking a molecular movie of bacteriorhodopsin



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

Pump lasers

	Ti:sapphire with OPA	Nd:YAG	OPO
Wavelength	200 - 2000 nm	532 nm	300 - 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) < 1 mJ (VIS)	<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)])	~150 μm[2)] (FWHM, Gaussian[3)])
		40 - 250 μm[4)] (through an optical fiber)	40 - 250 μm[4)] (through an optical fiber)
Experimental hutch	BL3 EH2	BL2 EH3	BL2 EH3
Remark		[1)] For optical-fiber option. [2)] Using plano-convex lens [3)] Optional: Top-hat beam profile [4)] Dependent on the fiber core size	