

5-4. SACLA Beamlines

1. Operation status

SCALA contains three beamlines (BL1–3), which are currently available for user operations^[1]. Table 1 summarizes the latest operational parameters of the beamlines. The soft X-ray free-electron laser (SX-FEL) beamline (BL1) has a dedicated 800-MeV linac to produce femtosecond SX pulses with photon energies of 40–150 eV^[2]. The two X-ray FEL (XFEL) beamlines (BL2 and BL3) are driven in parallel by the SACLA main linac, which can switch an electron-beam route in a pulse-by-pulse manner. Owing to the three-beamline operation started in FY2017, the user beamtime increased from ~4,000 hours in FY2016 to ~6,400 hours in FY2019.

In addition to the two XFEL beamlines, the main linac can provide a high-quality electron beam to the storage ring of SPring-8. Through elaborate injection tests in FY2018 and FY2019, simultaneous operations of SACLA and SPring-8 have commenced since April 2020. The parallel injection scheme slightly influences the operation of the XFEL beamlines, but it is not serious for most user experiments. SACLA suspends the XFEL operation for a while (roughly 10–20 min) during the beam injection to build up the electron charge in the SPring-8 storage ring. During the top-up operation of SPring-8, SACLA keeps the XFEL operation. An electron bunch is extracted from the 60-Hz bunch train and delivered to SPring-8 only a few times a minute.

The beamlines and experimental stations were upgraded through close collaborations with experts inside and outside the facility. Three strategic programs are ongoing to facilitate collaborative

R&Ds:

- (1) SACLA Basic Development Program
- (2) SACLA Industry–Academy Partnership Program
- (3) SACLA Research Support Program for Graduate Students

Here, the major upgrades of the beamlines and experimental stations in FY2019 are described.

Table 1. Major operational parameters of SACLA^[1].

	BL1	BL2 and BL3
Electron beam energy	800 MeV max.	8.5 GeV max.
Repetition	60 Hz max.	60 Hz max.
Undulator period	18 mm	18 mm
Undulator K value	2.1 max.	2.7 max.
Photon energy	40–150 eV	4–20 keV
Pulse duration	~30 fs	<10 fs

2. SX-FEL beamline (BL1)

2-1. Advanced focusing optics

A sub-micrometer focusing system for SX-FEL was developed in collaboration with Prof. H. Mimura (The University of Tokyo) under the SACLA Research Support Program for Graduate Students^[3]. A two-stage focusing scheme was adopted to construct an optical system with Kirkpatrick-Baez (KB) mirrors (first stage) and an ellipsoidal mirror (second stage). This system is currently being employed in user experiments.

The system was applied to a spatially resolved measurement of the magneto-optical Kerr effect

(MOKE) (scanning MOKE method). Figure 1 schematically shows the layout of the scanning MOKE experiment. The magnetic structures of an iron film were visualized with a resolution of 7 μm [4].

The two-stage focusing scheme was further developed for more advanced systems. Key optical elements are rotationally symmetrical mirrors with hollow shapes at the second stage. For example, a pair of hollow-shaped Wolter mirrors was used as the second-stage optics in a SX full-field microscope [5].

2-2. New experimental instruments

The SX-FEL beamline did not have common end-station instruments for specific experimental methods. Users had to bring their own instruments to perform their experiments. This style is

advantageous in accommodating the needs of diverse applications in the initial development stage of BL1. However, common-use instruments are necessary for efficient operations of experiments with well-established methods.

An ellipsometer for MOKE measurement was developed as a common-use instrument in collaboration with Prof. I. Matsuda (The University of Tokyo) under the SACLA Basic Development Program [6,7]. This MOKE instrument has multilayer mirrors for polarimetry of reflected light from the sample. These mirrors are switchable in a vacuum for resonant MOKE measurements at different photon energies [6]. In FY2020, the current system will be upgraded to a new one with a focusing mirror for incident SX-FEL and an in-vacuum sample changer.

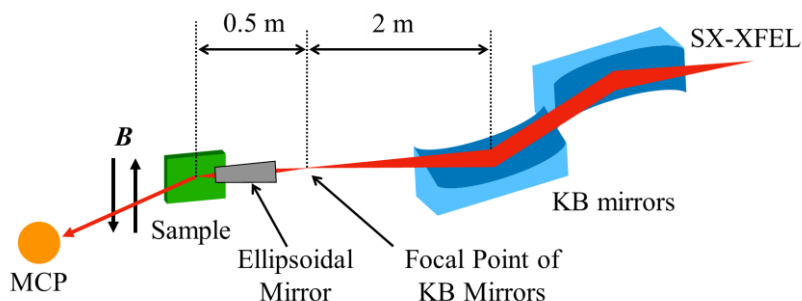


Fig. 1. Experimental system for a scanning MOKE method at SACLA BL1 [4].

3. XFEL beamlines (BL2 and BL3)

3-1. Instrument for coherent diffraction imaging (CDI) using a 100-nm XFEL beam

The Multiple Application X-ray Imaging Chamber (MAXIC) is an experimental instrument for CDI [8]. An advanced MAXIC (MAXIC-S) was developed for 100-nm focusing of the incident XFEL in collaboration with Prof. Y. Nishino (Hokkaido University). Multilayer KB mirrors can focus 4.0-

keV X-rays [9]. Due to the high photon density of the focused beam, sample images can be obtained with resolutions on the nanometer order. The MAXIC-S was installed at EH4b of BL2 in FY2019.

3-2. Experimental platforms with high-power optical laser systems

Since FY2018, experimental platforms equipped with high-power optical lasers have provided

additional research capabilities to SACLA users^[10,11]. The platforms are continuously developed for the studies on physical phenomena or material states under the extreme conditions produced by high-power lasers.

A long-pulse laser with a maximum energy above 50 J can excite a strong shock wave in a sample placed in a vacuum chamber at EH5 of BL3^[10]. The shock wave can compress a sample with a pressure above 100 GPa. XFEL probes the states of compressed matter via the X-ray diffraction (XRD) or small-angle X-ray scattering (SAXS) methods. XFEL can also capture ultrafast images, which show shock-wave propagation in matter. Since uniformity of the shock front is important in these experiments, diffractive beam homogenizers were developed in collaboration with Prof. N. Ozaki (Osaka University) with the support of the SACLA Basic Development Program. The laser pulse

focused through the homogenizer has a quasi-flat profile, which is suitable to excite a uniform shock wave.

A Ti:sapphire laser system, which delivers 40-fs optical pulses with a Joule-class energy, can produce high-energy-density states of matter at EH6 of BL2^[11]. Most experiments require a precise overlap in time and space. The timing jitter of the synchronization between the XFEL and the optical laser is equal to or less than the pulse duration (Fig. 2). In FY2019, an emission X-ray imaging system was installed on the platform to characterize the spatial overlap of the tightly focused lasers down to a few tens of micrometers or less. The system consists of a spherically bent quartz crystal to capture the monochromatic images of copper $K\alpha$ X-rays generated by the irradiation of intense-optical laser or the XFEL to copper foils.

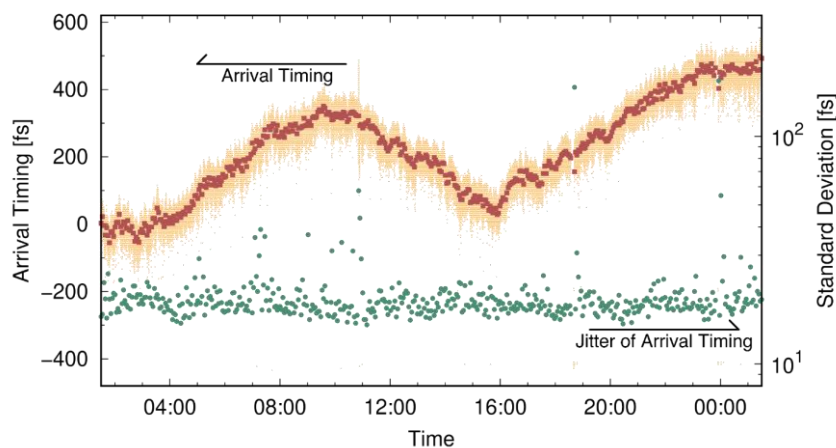


Fig. 2. Relative arrival timing of the high-power femtosecond optical laser to the XFEL (orange) and its standard deviation (green) corresponding to the jitter of arrival timing^[11].

4. Research highlights

4-1. Structure analysis of Photosystem II (PSII) in intermediate states of the water oxidation cycle

Professor J.-R. Shen (Okayama University) and

coworkers analyzed damage-free structures of PSII using ultrashort X-ray pulses of SACLA. For the five (S0–S4) in the water oxidation photocycle, they determined the structures of three intermediate states (S1–S3) using serial crystallography and

flash-cooled or ambient-temperature crystals [12,13,14]. These structures indicate a mechanism of dioxygen formation in photosynthetic water oxidation.

4-2. Ultrafast X-ray spectroscopy for tracking photochemical processes

Katayama and coworkers applied time-resolved X-ray absorption spectroscopy to explore ultrafast chemical processes in a photo-excited molecule on the femtosecond timescale [15]. They tracked the wavepacket dynamics associated with a bond-length change in a Cu(I)–phenanthroline complex. Their results demonstrated that ultrafast X-ray spectroscopy can provide deeper insights into chemical reactions.

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