5-4. SACLA Beamlines

1. Operation status

SACLA has been operated through FY2020 as scheduled except for the shutdown period due to the COVID-19 pandemic. Most experiments scheduled in the initial 2020A term were postponed to the latter half of the year. The rescheduling caused a significant reduction in user beamtime to ~3300 hours, which is about half of the previous years. Furthermore, nearly half of the international users canceled their experiments because of travel restrictions. Other international experiments were conducted mainly by collaborators based in Japan. The facility has started to develop a new remote scheme to increase remote capabilities and reduce loads of on-site collaborators. Remote users will be able to operate beamline equipment in pilot experiments under the scheme in late 2021.

Table 1 shows the operation parameters of the beamlines (BL1-3) at SACLA. BL1 is a soft X-ray (SX) free-electron laser (FEL) beamline using a dedicated linac. The other two beamlines, BL2 and BL3, are the hard X-ray FEL (XFEL) beamlines sharing the main linac. The beamlines can be operated simultaneously because the electron beam route is changed in a pulse-by-pulse manner by a fast-switching magnet. The electron beam has been injected constantly into the storage ring of SPring-8 since FY2020. The injection does not severely affect most experiments at SACLA.

Table 1. Major operation parameters of SACLA [1]

	BL1	BL2 & 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

As described in the following subsections, upgrades of beamlines and experimental stations have been conducted in FY2020. Some upgrades are outcomes of close collaborations with external experts under three strategic programs:

- SACLA Basic Development Program
- SACLA Industry–Academy Partnership Program
- SACLA Research Support Program for Graduate Students

2. SX-FEL beamline (BL1)

2-1. Beamline instruments

The one-photon ionization yield of argon is monitored as a nondestructive diagnostic of SX-FEL intensities at BL1. Here, argon ions are detected by an electron multiplier calibrated in collaboration with the AIST group [2] to obtain the absolute pulse energy. The calibrations were performed about every six months to compensate for the degradation of the detection efficiency of the detector. In FY2020, a compact radiometer was installed into the beamline to make the calibration easier and more frequent.

2-2. Experimental instrument

A sub-micrometer focusing system was developed for SX-FEL in FY2019 under the SACLA Basic Development Program and the SACLA Research Support Program for Graduate Students. The system is based on a two-stage focusing scheme using Kirkpatrick–Baez mirrors at the first stage and an ellipsoidal mirror at the second stage [3]. In FY2020, a Wolter mirror was adopted at the second stage, which made the alignment simpler and more robust. A new vacuum chamber has also been developed to use the sub-micrometer beam in user experiments. The commissioning and first user operation of this system will start in FY2021.

3. XFEL beamlines (BL2 and BL3)

3-1. Full auto-tuning of general beamline components at BL2 and BL3

Full auto-tuning software for general beamline components has been implemented at BL2 and BL3, facilitating the routine beamline tunings. The tunings had been manually conducted before every beamtime by two to three facility staff members. The newly developed software can finely adjust the photon energy of the XFEL, the optical axis after the offset mirrors or double-crystal monochromator, and amplifier gains for photodiodes in transmissive beam intensity monitors. The software will be officially released in late 2021.

3-2. Auto-tuning of *100exa* focusing system

A semi-auto-tuning system for the mirrors of the 100-nm focusing system (so-called “100exa”) [4] at EH5 of BL3 based on wavefront sensing has been introduced in FY2020. Manual tuning of the 100exa mirrors took over a few hours because of the strict tolerance for angular tuning and the difficulty in measuring focal properties. Moreover, frequent tunings every ~12 h were encouraged to maintain the focal properties.

The semi-auto-tuning is implemented through single-grating interferometry [5] using a 2D phase grating placed downstream of the focal point. At specific distances from the grating, periodic interference patterns (self-images) are formed through the Talbot effect. The wavefront error is reconstructed from the self-image through Fourier analysis and then expanded into a polynomial series. Each component can be linked to a parameter of the focusing mirror alignment, such as the incident angles, astigmatism, and perpendicularity of the mirrors. Finally, the mirrors are adequately tuned according to the wavefront error. The re-tuning of the mirrors can be completed within 5–10 min once the system is precisely calibrated.

3-3. Development of sub-10 nm focusing system

As part of the SACLA Basic Development Program, a new optical system for sub-10 nm focusing has been developed to produce an X-ray laser field with an intensity of ~10^{22} W/cm^2. An advanced Kirkpatrick–Baez (AKB) mirror geometry based on the Wolter-type III geometry [6] has been adopted since the AKB optics can reduce comatic aberration by satisfying Abbe’s sine condition, which leads to a wide tolerance to the incident angle error. The optical system has been developed to have numerical apertures of 0.01 and demagnification factors of more than 6000, which can attain a focusing spot size of ~8 nm at 9.1 keV. The optics were fabricated through the wavefront correction scheme [5] with an accuracy of λ/15 root-mean-square (rms), satisfying Maréchal’s criterion. The focusing test will be performed in FY2021 using the optics in a vacuum chamber at EH4c of BL3, followed by pilot experiments.

3-4. Timing stabilization of the femtosecond optical laser system for pump-probe experiments

A feedback system using a balanced optical-microwave phase detector (BOMPD) working at a

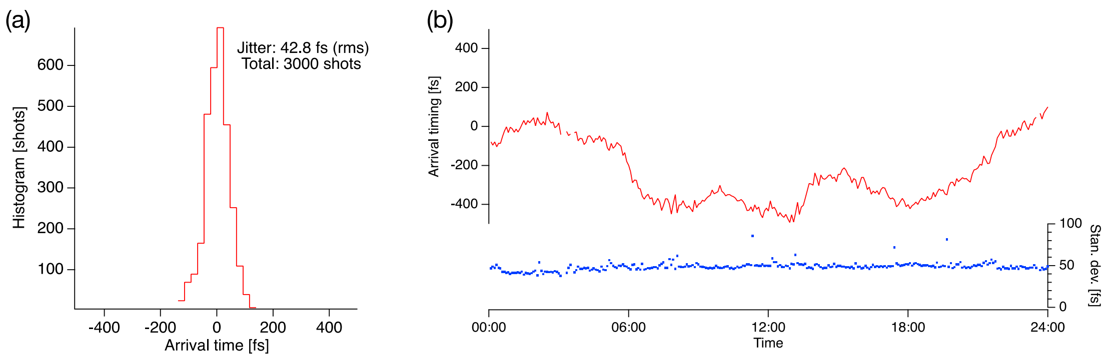

Fig. 1. Statistical data of the relative arrival timing between the XFEL and the sync-laser pulses: (a) histogram of 300 shots and (b) trends of averages (red) and standard deviations (blue) in 24 h [7].

C-band frequency (5.7 GHz) has been developed and installed in the femtosecond optical laser system (sync-laser) in LH1 for the precise time synchronization of the sync-laser to XFEL [7]. A relative arrival timing between the XFEL and the sync-laser using the new system based on the BOMPD is evaluated using the timing monitor installed in EH1 [8]. Figures 1(a) and 1(b) show a histogram of jitter and trends of averages and standard deviations in 24 h, respectively. Even though a long-term drift of ~0.5 ps remains in a day, the timing jitter is ~50 fs (rms), which is about one-sixth of the jitter previously reported using a commercial locking system equipped with a fast photodetector. As a demonstration of the advantage of the precise synchronization using the BOMPD, the time-resolved X-ray diffraction measurement of photo-excited bismuth (Bi) was performed. The coherent phonon in Bi was successfully observed without postprocessing for timing jitter mitigation [7].

3-5. Improvements of the experimental platform with high-power nanosecond optical laser

Experimental procedures have been much improved for experiments using a high-power nanosecond laser in EH5 at BL3. Many operators had worked at the same time in typical experiments because the equipment operations were not well systematized. However, such a style will not be suitable in the post-COVID-19 era. Users can now operate the equipment easily using an integrated command system developed in FY2020 for routine processes, for example, laser alignment and data acquisition.

The laser beam profiles at the focus have also been improved under a project of the SACLA Basic Development Program. The beam homogenization is crucial to excite uniform shock waves and create extreme states, which is one of the major topics at the platform. Three types of diffractive beam homogenizers with different spot sizes are available to make quasi-flattop profiles.

4. Research highlights

4-1. Contribution of double core-hole states to nonlinear multiple ionization

Fushitani et al. investigated the ultrafast multiphoton ionization of xenon in the intense laser fields by multi-electron-ion coincidence spectroscopy at BL1 [9]. They found that the pathway via the 4d double core-hole states of Xe makes a large contribution to the multiple ionization, despite the long FEL pulse duration compared with the lifetime of the 4d core-hole states.

4-2. Direct tracking of atomic motions during chemical bond formation using femtosecond X-ray solution scattering

Kim et al. applied time-resolved X-ray solution scattering to investigate ultrafast dynamics of photo-excited $[Au(CN)_2^-]_3$ [10]. They succeeded in tracking the trajectories of vibrational wavepackets during photo-induced bond formation between Au atoms on the femtosecond timescale. Their results demonstrate that the solution scattering technique using XFEL pulses can visualize atomic motions in chemical reactions.

4-3. Capturing atomic fluctuations with twin XFEL pulses

Shinohara et al. developed a method of characterizing the thermal fluctuation of materials [11]. Their method employs twin brilliant X-ray pulses generated by transmitting an XFEL pulse through the split-delay optics. By using water as a model sample, they demonstrated that one can access the timescale of atomic-scale thermal fluctuation by analyzing the visibility of the scattering patterns produced by the twin X-ray pulses. The new method should be highly useful for investigating atomic-level dynamics of condensed matters in a wide timescale from picoseconds to nanoseconds.

4-4. Structure determination of dopamine D2 receptor in complex with antipsychotic drug molecule by serial femtosecond crystallography

The human dopamine D2 receptor (D2R), which is a member of the G-protein-coupled receptor superfamily, is a key target of antipsychotic drug development. Im et al. have determined the structure of D2R in complex with the antipsychotic drug spiperone by serial femtosecond crystallography [12]. The structural information will be useful for designing novel antipsychotic drugs with few side effects.

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