

Breakout session A1: High-resolution and high-accuracy fs crystallography

Organizers: Ichiro Inoue & Kensuke Tono (SACLA)

Speakers: Ichiro Inoue (SACLA), Kiyofumi Takaba (RIKEN),
Hidetaka Kasai (U Tsukuba), Hiroshi Sugimoto (RIKEN)

1. Update plans of BL and instrumentations are presented from facility side:

- New standard configuration setup for crystallography (2θ up to 78 deg can be covered)
- New detector (CITIUS)
- Coating of transport mirrors at BL2 (cut off energy will be extended to 22 keV).

2. Representative users presented research highlights and requests to the facility:

- Organic compounds (SFX): Takaba
- Hard materials (SFX): Kasai
- Protein crystals (serial fs rotation crystallography: SF-ROX): Sugimoto

3. Round-table discussion (see next page)

Discussions

- **Critical photon energy for high-resolution fs crystallography**

- 20 keV ($d \sim 0.8 \text{ \AA}$ @ $2\theta = 45^\circ$) is sufficiently high in the present scientific cases.

- The users community and the facility should continue the discussion as a long term perspective.

- **Detector saturation in SF-ROX**

- The uses of CITIUS and/or higher photon energy might be a solution.

- In addition to the higher dynamic range, CITIUS has higher radiation tolerance than other X-ray CCDs such as MPCCD.

- **Weak diffraction signals in SFX of organic molecules at 20 keV**

- Facility staffs will try to improve the pulse energy by developing new tuning procedures for high photon energy beam.

- Detectors having single photon sensitivity (MPCCD & CITIUS) may improve the data quality.

- **Auto and fast alignment of the samples for high throughput measurements**

- As for SF-ROX, SACLA staff will consider the updates of the instrumentations in collaboration with SPring-8 team.

- For other methods, it would be nice to form collective opinions of the users' community.

- **Longer valid period of proposals (e.g., valid for 1 year)**

- Helpful for users to well prepare the experiment.

- Higher degree of freedom in planning experiments.