SACLA Users' Meeting
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Summary of the Ultrafast Chemistry Breakout Session

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Aim of this Breakout session

- Collect demands and proposals to SACLA from ultrafast chemistry users
- *e.g.*: Existing methods to be improved & new methods to be enabled
  - Measurements (scattering, XAFS, XES, RIXS,…)
  - Hardware (optical lasers, detectors, timing tool,…)
  - Software (data analysis on the fly, …)
  - Accelerator (two color, attosecond,…)

Methodologies (1/2)

1) Existing methods to be improved:

→X-ray scattering and diffraction, X-ray spectroscopies, i.e. XAS and XES, in particular EXAFS (?)

→Particularly, EXAFS and diffraction experimental capability should be enhanced at SACLA.

2) New methods to be enabled:

→Non-resonant valence-to-core XES, resonant XES, Inelastic X-ray Scattering, i.e. X-ray Raman…

→Regarding new photon hungry methods, SACLA will not compete with big machines (LCLS-II or European XFEL) directly.

Methodologies (2/2)

3) Exploit not only transverse coherence (imaging) but also longitudinal (temporal) coherence.
→ seeded pulses (transform-limited)
→ SACLA will try to develop a new scheme of self-seeding. For application, stable operation and easy tuning will be key points.

4) Include as many different techniques as possible
→ complementary observables will help to disentangle the electronic and nuclear degrees of freedom.

New pumping schemes (1/2)

Alternative schemes for “pumping” of chemical reactions:

→Going beyond the optical wavelengths! Only a small fractions of (bio)chemical reaction can be triggered with light...

→Bio-sample, dilute systems, using exotic lasers will be good examples to promote science at SACLA.

→Improve temporal resolution: measure jitter at the sample position (interferometric timing tool in liquid phase)

→Minimize GVM and optimize sample delivery for low dispersion of pump pulses.

→Use “exotic“ lasers (Yabashi-san in his talk) to trigger the dynamics, i.e. mid-IR pulses, THz pulses, etc.

New pumping schemes (2/2)

→ Avoid excessive (vibrational) heating of samples by depositing too much (light) energy into the system → ground-state chemistry

Especially in pump-probe experiments,

Don’t underestimate the (optical) pump lasers!

On-line analysis

- Software improvements:

→ Data reduction and analysis on-the-fly

→ More user-friendly interfaces to dig into big data sets

→ On-line and off-line cluster access (before, during and after beam times)

→ Many aspects of “user friendliness” have improved over past 5 years

→ Further automation, or easy analysis is sometimes very important and frequently underestimated. We should keep this kind of development.

New accelerator operation modes

- New accelerator parameters:

→ two-color mode: X-ray pump/X-ray probe experiments

→ Extremely ultrashort pulses → sub-5 fs down to sub 1-fs (attosecond)

→ Wavelength tunability in the hard X-ray range (unchallenged)

→ broadband X-ray pulses

→ single-shot dispersive XAS

→ higher repetition rate (not necessarily burst-mode, 1 kHz CW)

→ Let's think about submitting proposals to apply X-ray pump and x-ray probe experiments using different color.

SACLA-Spring-8 campus offers unique opportunities

- Joint SALCA and Spring-8 experiments:

  → SACLA/Spring-8 beamline
- 100-ps and ns-resolved experiments at Spring-8 before applying for XFEL beamtime. Preferential access to synchrotron beamtime as part of the XFEL-related projects is preferable.
- On-site optical spectroscopy laboratories to carry out complementary optical measurements
- Utility support is also important. We will keep this kind of developments.
- If the preferential access is difficult at SPring-8, we can collaborate with Adachi group at KEK and think to submit a proposal to PF-AR.

List of participants

- Yuichiro Kida (JST)
- Wojciech Gawelda (EXFEL)
- Andreas Galler (EXFEL)
- Tadashi Togashi (JASRI)
- Kyo Nakajima (JASRI)
- Hiroyuki Shimada (KEK)
- Tetsuo Katayama (JASRI)
- Shin-ichi Adachi (KEK)