High Energy Accelerator Research Organization (KEK)
Institute of Materials Structure Science (IMSS)
Photon Factory

Photon Factory SAC Time-resolved science subcommittee February 15-16, 2012

Executive Summary and Closing Remarks (final)

Robert Schoenlein, subcommittee Chairperson

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SAC Time-Resolved Science Subcommittee Members

SAC Subcommittee Meeting – February 15-16, 2012

Dr. Robert Schoenlein (Chair, Lawrence Berkeley National Laboratory/Advanced Light Source)
Prof. Jun-ichiro Mizuki (Kwansei Gakuin University)
Dr. Christian Bressler (European XFEL)
Prof. Mamoru Sato (Yokohama City University)
Prof. Martin Meedom Nielsen (University of Copenhagen)*

*absent from Subcommittee on February 16, 2012

SAC Remarks

This was the first meeting of the Time-resolved science subcommittee for the Photon Factory SAC. The Time-resolved Science subcommittee thanks the PF management and staff for their excellent logistical support, arrangements, and planning for the meeting. The committee greatly appreciates the effort that the PF scientists and users have put into preparing material for this meeting. We enjoyed the stimulating scientific discussions, and the chance to hear about and tour the latest developments at the Photon Factory, and we very much appreciated the generous hospitality.

Question 1 – Are the scope and strategies of the time-resolved experiment group suitable in the domestic and the international contexts of SR research?

- The committee heard a general overview from Director S. Wakatsuki on activities at the Photon Factory, and a more detailed discussion on the PF-AR Upgrade and ERL Project from H. Kawata. S. Adachi presented an overview of the technical scope, science, and strategy for the PF-AR Time-resolved x-ray beamline NW14A. In general, the strategies of the time-resolved group are highly appropriate in the context of both domestic and international synchrotron research.
- NW14A is one of the very few beamlines worldwide that is dedicated to time-resolved science. The diversity of research (ranging from physical chemistry, to biology, to materials) and techniques (including both spectroscopy and scattering) is quite impressive. Juggling the breadth of research is difficult, but may be necessary in order to cultivate a broad user community that might drive the need for a future light source. A key element of the strategy is to cover a wide range of time-resolved x-ray applications rather than focusing on a single x-ray technique. In general, this seems to be a reasonable strategy, but there should be some limit on the breadth of applications, and a serious effort to try to judge in advance which applications might be the most promising.

Question 1 – Are the scope and strategies of the time-resolved experiment group suitable in the domestic and the international contexts of SR research? (con't)

- In order to maintain some breadth of applications, without sacrificing too much productivity, an upgrade of NW14 to streamline the switching between operating modes (broad-band vs. monochromatic), and to reduce the manpower requirements for experimental set-up and alignment are advised. Beyond that, increasing the number of PF-AR and PF time-resolved beamlines (each specialized for specific techniques), would be desirable, and could help make the case for an ERL by establishing a strong user community.

- The committee recognizes that this may be limited by manpower and funding. A novel University/KEK partnership model was proposed as a means for securing a net increase of funding for both universities and KEK, rather than diverting it from universities to KEK in order to establish a network of partner university outstations at KEK. This certainly will include the time resolved experiments as part of the roadmap for the 3GeV ERL. The committee is very supportive of this approach.

Question 1 – Are the scope and strategies of the time-resolved experiment group suitable in the domestic and the international contexts of SR research? (con't)

- The ERL developments at KEK are at the forefront of efforts worldwide. The compact ERL should be a valuable stepping stone (both scientifically and technically) to the development of a future ERL light source. Since funding and manpower are somewhat limited, it may be advisable to focus efforts more sharply on science that requires (and can truly exploit) the MHz repetition rates, while also capitalizing as much as possible on the strong local user communities. This may help build the science case, and the user base for an ERL as a high repetition rate light source.

- Recently, the preliminary upgrade plan of SPring-8 was published. It is important to rationalize the ERL project in the context of the SPring-8 upgrade plan, while emphasizing the complementarity of the sources. Some of the elements of the SPring-8 upgrade plan that may relate to (or overlap with) the ERL project include the emphasis on diffraction-limited x-ray beams (due to lower e-beam emittance), the potential for short pulses (at the picosecond level), and time-resolved experiments combining SPring-8 with SACLA. Emphasis on the differences from the SPring-8 upgrade plan may be important to show the scientific and technical significance (originality, uniqueness, etc.) of the ERL project.

Question 2 – The BL instrumentation and user operation

A) Are the scope and strategy of BL instrumentation developments satisfactory?

- The committee heard a detailed discussion on strategy and instrumentation development for the PF-AR time-resolved x-ray beamline from S. Adachi. These include top-up operation with direct injection at 6.5 GeV, emittance reduction, development of smaller x-ray focus, and a new laser system to support MHz experiments.
- The committee strongly supports this strategy. Top-up and direct injection at 6.5 GeV will have a big impact on the productivity of the facility, and is a big advantage over the present ramped energy operation. Emittance improvements, better focusing optics, and a new laser system will enable MHz experiments which will provide the scientific and technical foundation for an ERL. Given the PF-AR source characteristics, capillaries were proposed as the most effective approach for focusing to small spot sizes. The committee suggests that Be lenses also be considered.

Question 2 – The BL instrumentation and user operation

A) Are the scope and strategy of BL instrumentation developments satisfactory? (con't)

- One missing element in this strategy is high speed detectors. In this area, Photon Factory may be able to capitalize on developments at other labs, as higher speed detectors are a general need for future high repetition rate light sources. Gated detectors may provide some flexibility in choice of pump/probe frequency according to the needs of specific experiments. Measurements at adjustable rates from kHz to MHz would be highly desirable, as well as including more x-ray techniques to the tools available, e.g., the scientific impact of solution-phase scattering experiments may be enhanced by simultaneous XES with WAXS.

B) Staffing issues: Is the level of user supports sufficient?

- The PF-AR time-resolved activities benefit from a very dedicated and creative scientific staff, as well as a close collaboration between staff and users. While the staffing level may be less than ideal, this working relationship helps to bridge the gap.
- As the user community grows and broadens (including less-experienced users), increased staffing will become necessary.
- With limited resources and manpower, it may be advisable to prioritize time-resolved activities towards those that are likely to have the greatest impact on making a scientific case, and building strong user advocates for a new ERL light source at KEK.

C) Are we open enough to overseas users?

- The current 50/50 ratio appears unusually open to scientific users from the international community. This reflects the rather unique capabilities of NW14.

- Arguably a more important question may be which scientific users will be most helpful and influential in making the case for a new light source at KEK. Some international users will be important, but a strong local contingent, funded through Japan science agencies, should be very influential advocates for an ERL facility.

D) Cooperation and Complementarity with SPring-8 and others?

- S. Adachi has been an important link to SPring-8 and other facilities. In general, it is valuable for PF scientists to have an opportunity to participate at some level in research activities at other light sources. With the emergence of FELs and SACLA, it is important for scientists to be familiar with the capabilities (and limitations) of these facilities, the new time-resolved experimental techniques, and science applications in order to help identify areas where a new light source could be complementary.

Question 3 – Assessment of science outputs from users (including the level and impacts of scientific presentations)?

- The committee heard very interesting science from PF-AR users, particularly the work of S. Koshihara's group on cooperative photo-induced phase transition, the work of Y.C. Sasaki on diffractive x-ray tracking of individual single protein motions, and the work of S. Nozawa on FeII(phen) spin crossover compounds and on Fe-Co cyano complexes. S. Adachi also presented a number of additional user highlights from NW14, including a scattering study of bond changes of molecules in solution.

- NW14 has been in limited user operation since mid-2007, and open to general users only since 2009. In this short period, the beamline has established an impressive record of scientific productivity, covering a broad range of science (and techniques), with a number of high-profile publications (PNAS, PRL, Nature Materials).

- To the extent that new users are recruited and new science areas developed for NW14, these efforts should encourage users and focus on science areas that will help make the case for an ERL facility – particularly approaches that can exploit the high repetition rates that are unique to ERLs.

Question 4 – Future prospects. How do you evaluate these plans?
A)Development of the time-resolved soft X-ray applications by means of hybrid operation at PF.

- S. Adachi presented a strong plan to implement hybrid operation at PF and exploit this for time-resolved science ranging from spin dynamics of magnetic thin films to surface chemical reactions, to photo-induced phase transitions etc. This operating mode is similar to those (hybrid and/or camshaft) now in routine use at other synchrotrons worldwide.

- Candidate beamlines such as BL-2A and BL-16A have been identified, and the committee recommends further development of this strategy and careful consideration of the most effective target beamline(s). Plans for a mobile high repetition rate laser system are currently under discussion, and the committee looks forward to hearing further details

- Gated detectors should be considered, and are a particular challenge for science requiring 2D detection (e.g. scattering/imaging). Ideally users should be able to choose the optimum repetition rate for specific experiments (kHz to MHz).

Question 4 – Future prospects. How do you evaluate these plans?
A)Development of the time-resolved soft X-ray applications by means of hybrid operation at PF. (con't)

- Dedicated manpower will be needed at PF to make this operating mode successful (laser support, data acquisition, user support etc.) – particularly depending on the expertise of the user. Involvement of existing beamline scientists at PF is recommended as a means to expand PF expertise in time-resolved x-ray science.

- One recommendation is to identify key user groups (with some expertise) that can help drive this development. The current user groups of NW14 may be good starting points for this.

B) Measurement of high repetition rate (upto 794 kHz) at PF-AR

- S. Adachi presented strong plans for high repetition rate operation at PF-AR. These included emittance reduction, development of smaller x-ray focus, and laser system to support MHz experiments. The committee strongly supports these plans as they are an essential step in developing the science, measurements techniques, and user community that will drive the development of an ERL facility at KEK.

- Projected performance is competitive with similar facilities worldwide (e.g. ESRF ID9/26 and APS Sectors 7/11) operating in hybrid mode. A distinct advantage of the PF-AR operating in single bunch mode is that gated detectors or chopper systems will not be necessary for experiments exploiting the full repetition rate.

C) Femtosecond time-resolved experiments by means of cERL and XFEL to introduce the science case of ERL

- Current focus on inverse Compton and THz at cERL are very interesting, but these are primarily source development efforts, and are technically very challenging in their own right. Is there sufficient manpower for this activity? Are there plans to have an EUV undulator (possibly superconducting with short period) once the full cERL is operational? What photon energy range could such a source cover, and what might be initial science applications?

- (Answer from the PF)
  - Although the manpower is always limited, some designated members of the Photon Factory staff are supposed to participate in the cERL project. In fact, Dr. Nozawa, so far employed as a limited-time contract assistant professor, has been promoted to tenured associate professor and is expected to lead the science experiments on the cERL.
  - Installation of EUV undulator at cERL is not planned at the moment. If an undulator with 32-mm period length is installed in the 100-MeV cERL, the 1st, 3rd, and 5th harmonics will cover 0.5-10 eV region.

C) Femtosecond time-resolved experiments by means of cERL and XFEL to introduce the science case of ERL (con't)

- A parallel effort should be made on detailed plans for initial science experiments using cERL. This will be important to persuade KEK, the user community, and funding agencies to eventually construct a 3GeV ERL. This effort should focus on science requiring high rep-rate and/or coherent soft x-rays, and/or nano-beams and other key unique capabilities of an ERL. For example:
  - Photo-emission electron microscopy (magnetization dynamics)
  - Time-resolved photoemission spectroscopy (TR-ARPES) – also with hard x-rays, core levels
  - Spin-resolved ARPES
  - Coherent diffractive imaging, phase contrast imaging
  - THz pump, x-ray probe experiments