Report from the Meeting of the Photon Factory SAC Materials Chemistry Subcommittee

February 21-22, 2011

Materials Chemistry Subcommittee Members:

Y. Iwasawa - Chair / University of Electro-Communications
K. Janssens - University of Antwerp
M. Newville - University of Chicago
S. Pascarelli - European Synchrotron Radiation Facility
M. C. Ridgway - Australian National University
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*absent from Subcommittee on February 21-22, 2011

Participants from PF:

Osamu Shimomura (Director of IMSS)
Soichi Wakatsuki (Director of PF)
Kenji Ito (Head of Synchrotron Radiation Science Div. 1)
Masaharu Nomura (Head of Synchrotron Radiation Science Div. 2)
Yukinori Kobayashi (Head of Accelerator Div. VII)
Hiroshi Kawata (Head of ERL Project Office)
Youichi Murakami (Head of Condensed Matter Research Center)
Atsuo Iida (Head of Materials Chemistry Group)

Question 1 – Are the scope and strategies of the materials chemistry group suitable in the domestic and the international contexts of SR research?

Third generation sources have an advantage concerning brightness, but PF is competitive in view of sample environments, and timing experiments, especially for bulk XAFS.

A) XAF

At the XAFS and its related beamlines, nearly 200 programs are running and nearly 120 papers are published in each year. This group also accepts non-XAFS experiments such as AXS, RXES, SAXS and XRD.

Catalysis work at PF, especially using time-resolved XAFS (QXAFS or DXAFS) is particularly well developed and supported. Fundamental and applied material sciences and environmental sciences are equally addressed. There is a healthy balance between XAFS at PF and that at other facilities in Japan, and this balance should be maintained. Many new instrumental developments have come from PF in the area of XAFS.

Micro-EXAFS with 10-20 μm beam size at the new BL15A will be valuable in many fields of science. For the new beamline, combination with complementary *in-situ* techniques is seen as an important development.

B) X-ray fluorescence analysis (XRF) / microbeam analysis

Number of proposals is nearly 30 per year. Research fields cover various analytical applications. Micro-SAXS is the other application of the BL4A micro-probe.

The 4A micro-XRF beamline is a relatively old facility, but the PF staff and users have made their best efforts to fully exploit its microbeam capabilities in a variety of disciplines. Given the emittance available, the current optics and beamline make the best use of the facility to obtain optimal spatial resolution.

Question 2 – The BL instrumentation and user operation

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

- XAFS

  There are 4 stations using bending magnet source at PF. They are 12C(high photon flux, versatile), 9 A(high photon flux, Soft X-ray mode, 2.1 keV - 5 keV), and 9C (XAFS and SAXS/WAXS), 7C (XAFS and its related science, will be closed).

  And there are 2 stations at PF-AR as written below.

NW2A (Tapered Undulator, DXAFS and others), NW10A (high energy).
DXAFS at NW2A, QXAFS at some stations, and SX (soft X-ray) mode at BL9A have been successfully developed.
In-situ time-resolved experiments are actively carried out. Developments of many instruments, including a double crystal monochromator, control system, sample environment, optical equipment, and software have been made.

- XRF/microbeam (BL4A)
  Several types of SRXRF/XANES systems have been commonly used. R & D has been carried out continuously.

We emphasize that in-house development is well appreciated, especially given the limited staff.

Development of more efficient detectors is a critical issue at all synchrotron sources. Looking to new detector technologies would be an important step. Pursuing collaborations within KEK or external research partners is recommended.

PF should provide some other analytical capabilities, either off-line or on-line, for the users with the cooperation of the user community. For example, *in-situ* UV, IR, XRD, or Raman systems would be attractive for operando XAFS experiments.

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

The XAFS group consists of three staff full-time members, three staff concurrent member (including Prof. Nomura), and one full-time member for industrial use.

The low staffing level is a serious problem. Having an average of 2 staff (one scientist and one technician) for user support per beamline is recommended. This is still well below the international standard, which is typically 3 or 4 staff at European and North American synchrotron facilities. Having increased staffing levels would continue the PF commitment to excellence in user support, education, and expanding the user base to new and emerging applications. It would also foster in-house development of cutting edge science, and allow PF - to remain competitive with international facilities. This should be viewed as optimizing the investment already made in PF and PF-AR, and planned for future machines at KEK. Investing resources in recruiting and educating young staff for these future light sources is vital.

NW2A is a unique instrument, and its use for time-resolved XAFS should be

promoted. Internal mobility of staff and collaboration within PF or with outside groups could provide a way to develop this specific capability into a stable facility for users.

C) Is the balance between academic and industrial use appropriate?

It now reaches 20 % of the total XAFS beam time. Materials Chemistry group is involved in a MEXT program: Open Advanced Research Facilities Initiative. The industrial usage of micro-analysis is modest.

The limit of beamtime for industrial users is set to 20%. This limit could be increased for XAFS, to 25% or 30% in this field, without seriously impacting the availability for academic research, especially given the current proposal approval rate. A slight increase in industrial use may alleviate some staffing issues.

D) Are we open enough to overseas users?

(XAFS) The number of proposals from oversea institutes is about 8% in average for the last 10 years. It is more than 20% in the previous year reflecting the cooperation of PF in helping Korean users who need beamtime during the long shutdown of PAL.

(XRF) 10% to 15% of the XRF proposal is from abroad, mainly from China.

PF is open to oversea users, especially for XAFS.

E) Cooperation and Complementarity with SPring-8 and others

PF is complementary with SPring-8, especially in single bunch experiments at PF-AR, and by providing ample beamtime for bulk-XAFS work. If the staffing levels could be improved, the ability to cooperate with SPring-8 and international facilities would increase. In particular, the micro-XRF work at PF complements the BL37XU microprobe at SPring-8.

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

- About 120 papers (XAFS) are published annually.
  13 XAFS related papers were published in the high Impact Factor journals (IF>=8).
  Prof. Iwasawa's group published 7 papers (catalysts) and six other groups published one paper each.
  From NW2A, Prof. Fujita's and Prof. Iwasawa's group published 16 papers

(XRD) and 2 papers (catalysts), respectively, in the high Impact Factor journals.

- 14 papers from BL4A (XRF/μ-beam) on average are published annually during the last 10 years. 8 papers were published in journals with IF>=4 for the last 5 years.

The scientific output from the XAFS and microprobe beamlines at PF is excellent, especially in comparison to other 2nd generation sources, and given the staffing levels.

The high impact of the catalysis XAFS work is very impressive. Increasing the staffing levels, especially targeted to specific fields (catalysis, environmental science) that could implement complementary *in-situ* techniques would further increase the output of the PF XAFS beamlines.

Question 4 – (XAFS) External grants: is the future secure? How much should we expand industrial use?

The usage fee covers most of the budget (60% -95%) needed for the maintenance and upgrade of the XAFS related beam lines.

Encouraging and enabling PF staff to seek additional funding is recommended.

External funding may be the best way to increase limited-term staffing levels, which could then allow senior staff to seek support for additional permanent staff within KEK. External grants also promote the research profile of the grantee and the institution.

Question 5 – Future prospects. How do you evaluate these plans?

a) New short gap undulator microfocus BL15A
b) Extension and refurbishment of BL12C
c) BL9C dedicated to XAFS
d) BL7C shutdown
e) Future light source

New BL15A will expand the capabilities of PF and provide excellent opportunities for combined micro-XRF, micro-XAFS, and micro-XRD. This beamline will also have micro-SAXS capabilities. All of these techniques should be allowed to fully develop at this beamline before allowing user demand to dictate the allocation of beamtimes.

This new beamline should have dedicated, additional scientific staff.

BL12C is planned to increase the hutch size to allow *in-situ* gas flow sample environments, and also to add a conical collimating mirror before and a conical focusing mirror after the DCM. This will result in a better use of the BM source, which will further improve this beamline. Looking into new fluorescence detectors

with higher count rate should be done as well. The level and quality of sample environments should be improved accordingly, which requires a strong collaboration with user communities.

The panel endorses the plan to dedicate BL9C to XAFS experiments (to the exclusion of SAXS) in accordance with the operation of new BL15A which will simplify the overall operation.

Proposed shutdown of BL7C when BL15A is brought on-line is reasonable considering the hardware of the beamline and the staffing situation. We acknowledge the additional burden to staff in swapping XAFS and RXES setups. The shutdown may eliminate the RXES capabilities at PF. This should be carefully discussed with the users and be evaluated by the SAC in terms of the scientific strategy of the facility.

For future light sources, installing undulator beamlines at KEK-B and an ERL are both being pursued at KEK. These strategies for low emittance machines are very important for all photon science areas in Japan. This will offer a major advance for micro- and nano-analysis, including micro-XAFS and sub-micro-XAFS in two and three dimensions. Whether the new facilities are particularly suited for chemical characterization with standard, bulk XAFS is not certain, but this will remain an important need for research.

ISAC Materials Chemistry Subcommittee

Feb. 21(Mon), 2011

09:00-09:05 Welcome (O. Shimomura)

09:05-09:40 Photon Factory and Charge to the subcommittee (S. Wakatsuki)

09:40-10:40 XAFS I Overview (M. Nomura） 50 min + 10 min

10:40-10:55 Coffee break 15 min

10:55-12:00 XAFS II

a. BL-12C & NW10A (H. Nitani) 20 min

b. BL-9A & NW2A (H. Abe) 20 min

c. BL-7C & BL-9C (M. Nomura) 10 min

Discussion 15 min

12:00-13:00 Lunch

13:00-13:25 XRF/microbeam (A. Iida) 20 min + 5 min

13:25-14:35 Science highlights I (30 min + 5 min) x 2 = 70 min

3 dimensional structure analysis on the metal clusters on oxides.

- the investigation on the metal-support interaction for the control of the structure of surface species (Prof. K. Asakura, Hokkaido University)

Application of SR-XRF to Environmental,Forensic and Archaeological Sciences. (Prof. I. Nakai, Tokyo University of Science)

14:35-14:50 Coffee break 15 min

14:50-16:05 Site visit and discussion individually with PF staff

16:05-16:20 Coffee break 15 min

16:20-17:30 Science highlights II (30 min + 5 min) x 2 = 70 min

Molecular Environmental Geochemistry: linking microscopic and macroscopic phenomena by X-ray absorption spectroscopy

(Prof. Y. Takahashi, Hiroshima University)

Magnetic and film structures of CO, NO adsorbed Fe/Cu(001) thin films observed by depth-resolved XMCD and EXAFS (Prof. H. Abe, KEK)

17:30-18:00 Discussion <Closed Session>

19:00- Dinner

Feb. 22(Tue), 2011

09:00-10:00	Discussion <Closed Session>
10:00-11:30	Time for writing a preliminary report <Closed Session>
11:30-12:00	Summary presentation