

Photon Factory Science Advisory Committee Review of Material Science Section Summary July 1, 2020

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Based on the reports and presentations, I would like to answer the following questions raised by the director of IMSS, Dr. N. Kosugi.

Answers to general questions:

1. How does the SAC evaluate the present status of the Mater. Sci. Sec.?

Researchers within the Mater. Sci. Sec. are doing an excellent job both in terms both their own research activities and developing advanced synchrotron techniques. The Mater. Sci. Sec. has an important dual role in both developing their own science and techniques as well as bringing these developments to wider use for the user community. Having this dual role allows for staff to have necessary freedom to move between the continuum of science and technique development, based on staff interest/background and the needs of the group in terms of user support. This is important for staff career growth as well providing positive feedback for user groups. It also allows the group to be responsive to developing trends and immediate societal needs, such as a Covid-19 related research which they have contributed to recently. Several examples of the value of this dual role is given by the research and developments noted below.

Answers to general questions (cont.):

It should be noted that the Mater. Sci. Sec. is operating in relatively constrained conditions, namely a limited budget, relatively old facility (oldest synchrotron in Japan and nearly in the world) and limited human resources. In particular, the staffing levels for beamline support are on the order of one person per beamline, which is significantly lower than for other facilities worldwide (typically three or higher). This has some obvious limitations on ability of staff to develop new instrumentation/techniques and potential overwork for the staff. It is therefore important to consider additional support for the beamlines, either by deciding to consolidate beamlines, providing higher levels of funding and/or making operations more efficient. To this point, the recently formed Center for Integrative Quantum Beam Science represents a promising way to enhance the budget, as well as provide a unique integrated suite of techniques for materials evaluation.

Answers to general questions (cont.):

2. How does the SAC evaluate research projects in the Mater. Sci. Sec.? Are these research outputs adequate?

The Mater. Sci. Sec. has strategically chosen several areas to develop their research, which include studies of chemical and mechanical heterogeneity, surfaces/interfaces and time-resolved processes. For each of these areas, the Mater. Sci. Sec. has pursued science aims to resolve long-standing questions in the field. For heterogeneity, in-situ imaging studies of carbon-matrix composites and EBCs have demonstrated world-leading spatial resolutions to study chemical and mechanical heterogeneity. Such studies provide information needed by industrial partners to reduce weight and engine efficiency in aerospace materials. Similarly, iron-ore studies have revealed the distribution of iron-oxide phases with respect to porosity, which is important information for steel-manufacturers. The time-resolved research has been used to study dynamic processes including artificial photosynthesis, photo-chemical reactions and shock-induced deformation with world-leading time resolutions. Through the development of time-resolved surface XAFS (TREXS), several surface catalytic processes have been revealed, leading to several publications and grants.

For the 2013-2020 (partial) period, the total publications by Mater. Sci. Sec. members is 168 which represents about 20% of the publications at the group-supported beamlines which average about 100 publications annually. Many of these publications are in high-impact materials science journals (e.g. Nat, Nat Comm, PRL, JAP) and the publication rate is considered strong, and indicative of high and consistent scientific output by Mater. Sci. Sec. and users they support.

Answers to general questions (cont.):

3. How does the SAC evaluate the recent developments of facilities in the Mater. Sci. Sec.?

There are several exciting developments within the research facilities operated by the Mater. Sci. Sec.. These include development of new techniques, such as TREXS for studying surface/interface properties, time-resolved spectroscopy and diffraction to study irreversible processes and multi-scale in-situ studies including nano-CT under applied load. Total reflection x-ray spectroscopy (TREXS) is a new surface sensitive method developed within Mater. Sci. Sec. which has been used to study catalytic processes with both academic and industrial partners. It could be expected that TREXS will be used at other synchrotron facilities as well in coming years. The time-resolved work leverages the unique properties of the PF-AR facility for high x-ray energy, high-flux, and single-bunch experiments. Through instrumentation developments (laser systems and electronics), Mater. Sci. Sec. scientists have developed ns-ps resolution capabilities for both XAFS and diffraction measurements, which are of great interest to materials science researchers studying dynamics. Ongoing efforts to couple these experiments with those from free electron lasers, to provide a wide time range (fs- μ s) to observe dynamic processes are encouraged. In-situ loading capabilities developed for investigating crack formation in composites and chemical speciation in environmental barrier coatings (EBCs) at the nano-scale level are world-leading in terms of resolution. Use of such multi-scale and multi-modal probes to investigate a single sample in-situ at one beamline (as opposed to moving the sample between specialized beamlines) is an ongoing trend at many synchrotron beamlines worldwide, and such developments are encouraged to continue at the Photon Factory and be supported at Mater. Sci. Sec. beamlines in particular.

Answers to general questions (cont.):

4. How does the SAC evaluate the funding situation of the Mater. Sci. Sec.?

According to the provided information (Fig. 5.1.1. in the activity report), the budget provided by IMSS for the group is limited to a small fraction of the overall budget, and this fraction has decreased rather steadily from FY13-19. To supplement this budget, the Mater. Sci. Sec. group is carrying out cooperative research projects with several private companies and pay-by-time use. The amount of and funding level for such projects is impressive, important and should be pursued strategically. However it should be considered that the IMSS not be over-reliant on them for funding, as they can require extensive time and energy to create – which competes with the staff's need to complete core activities (research and user support). Here some consolidation of beamlines across the Photon Factory facility may help the operating funding burden (if same funding, this would provide more funding per beamline) as well as provide the opportunity for strategic investments (e.g. robotics for sample changing, in-situ equipment, detectors, etc.).

Answers to general questions (cont.):

5. How does the SAC evaluate the relationship with industries?

The Mater. Sci. Sec. has several existing collaborations with private companies, which include heavy industries (e.g. steel makers), transportation and electronics. This is reflected in the large number of grants they are involved with, many of which involve industry (Table 5.1.1 in report). They have provided key research results on materials as part of the 'Structural Materials for Innovation' national project which involves a lot of major companies. Such collaborations are very important to understand needs in industries and provide positive feedback to industries on new materials and/or processes as well as deeper understanding of existing materials.

Answers to general questions (cont.):

6. Is the Mater. Sci. Sec. moving in the right direction? Are the future development items adequate?

Scientifically the Mater. Sci. Sec. has chosen several key areas to pursue, which as noted above are considered good choices based on their wide breadth and societal and industrial impact. The Mater. Sci. Sec. is pursuing many developments which should put them in strong position in the future. One of these is developing automated, high-throughput measurements, particularly for XAFS. They have implemented many fly-scanning techniques for faster data measurement, with plans to increase these activities further (implement for more scans and at more beamlines). They are also starting to apply information technologies and advanced algorithms to handle big data, such as obtained by multi- dimensional XRM data. These activities should be supported, noting that the speed and number of the developments would increase (and maybe in many cases only be possible) if the number of staff per beamline increase. Management may consider evaluating these areas on a more regular basis than 5 years (perhaps on the range of every 3 years) given the rapidly evolving nature of science and technology at present.

Answers to specific questions:

7. How does SAC evaluate the leadership of the Mater. Sci. Sec. in the field of materials science? Has the Mater. Sci. Sec. supplied facilities and research environment that are essential for materials science research?

The Mater. Sci. Sec. is providing good strategic leadership in many materials science areas. Examples include their development of automated and high-throughput measurements for XAFS, leading time- resolved research and multi-scale, multi-modal studies of heterogeneity. The Mater. Sci. Sec. has a dedicated in-house CT unit which is helpful to measure larger-scale materials, complementing the nano/micro-scale synchrotron studies. This can be particularly important to industry, who often have larger samples they do not wish to cut and for which coarser, larger field of view scans provide a good starting point/justification for more detailed synchrotron measurements. Outreach activities are strong, particularly in the area of educating students and providing specialized workshops to address the needs of users. By continuing to share their knowledge and instrumental and technique developments with users, the group promises to positively impact the materials science community for years to come.

Answers to specific questions (cont.):

8. Does the Mater. Sci. Sec. have potential to play a role of an international academic research center?

The Photon Factory is already playing a strong role in the field of materials science internationally, though it is relatively old facility and the budget and human resource is limited. The Mater. Sci. Sec. provides both scientific and technical leadership within several Photon Factory beamlines, and their dual roles should continue in order to provide the most benefits to the scientific community worldwide. It is important that the Mater. Sci. Section both follow important science trends and maintain a good relationship with corporations, as well as educate young students and researchers. They appear to have been doing a good job in these respects over their evaluation period. More broadly, they should play an important part in the CIQuS initiative, which will harness four distinct probes operated by the IMSS (photon, neutron, muon, and positron) to evaluate/modify materials. As such coupled facilities are very rare, the Mater. Sci. Sec. could take a leading role in researching ways to couple these probes in order to obtain key materials information.

Answers to specific questions (cont.):

9. How does SAC evaluate the PR activities?

The Mater. Sci. Sec. appears to be doing a good job with outreach to several communities. This includes industry, graduate students and other synchrotron facilities. The facility is taking on the important role of training graduate students, which will allow Japan to continue to provide a strong synchrotron presence worldwide. Examples include a special proposal for new students (T-type) and special course of the CUPAL program. The group has hosted several workshops over the evaluation period to evaluate users needs and perspectives, particularly in relation to potential new/renovated beamlines or scientific directions, with at least some coordination with other synchrotron facilities within Japan. Their efforts to develop round-robin 'standards' and databases particularly for XAFS are notable as they provide consistency checks for users. The Mater. Sci. Sec. group maintains several websites (e.g. <https://www2.kek.jp/imss/eng/>) which are up to date and contain both relevant scientific highlights and facility details that potential users may be interested in. Whether the group's activities and impacts have penetrated into mainstream society is difficult to judge. If this latter point is important, more support by dedicated PR staff could be useful as it is difficult for scientists to do this alone. Many light source facilities (e.g. ESRF, APS) have full time staff for these efforts.

Answers to specific questions (cont.):

10. Any valuable comments for the future perspective of the Mater. Sci. Sec.?

The PF in general, should take a closer look at the number of beamlines it is supporting and consider if all are needed or can be consolidated, given the limited staffing. Maintaining the dual roles of researchers and beamline support for staff within Mater. Sci. Sec. is important for providing flexibility to address (often evolving) needs within the section. This flexibility is especially important given the relatively low staffing for beamline support, to allow for 'surging' (putting 2 or more people on upgrades for limited period), ensuring some overlap in expertise (e.g. if one person is sick, that others can help out at their beamline) and can help staff morale (part of a large team which works together).

One area which could benefit the Mater. Sci. Sec. and photon factory in general is increased collaborations with specialists in data acquisition, data handling and computational science. While it can be difficult to find and hire staff who have both some synchrotron as well as computer science background, they can have a wide influence on efficiency at the facility. For example, examining the opportunities of AI and robotics for sample changing may help alleviate some of the workload among staff – noting however that significant efforts are required to set these capabilities up. The activity report shows that the Mater. Sci. Sec. has started these activities and that I believe that they should continue to focus on these areas. This trend is increasing at synchrotron facilities worldwide, so increasing support through new dedicated staff and/or part time consultants should be strongly considered in the near future.

(end of the review summary)