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

Report from the 2nd Meeting of the Photon Factory International Science Advisory Committee (ISAC)

March 4-5, 2008

Introduction, ISAC Process and Report Organization

The Photon Factory International Science Advisory Committee (ISAC) was chartered by the Institute of Materials Structure Science (IMSS) of the High Energy Accelerator Research Organization (KEK) with providing ongoing advice on the operations and strategic planning for the Photon Factory (PF). The ISAC meeting on March 4-5, 2008 was the second meeting for this Committee.

ISAC was provided written information, including copies of many of the presentations, in advance of ISAC meeting that was held in Tsukuba, Japan at the Photon Factory on April 4-5, 2008. ISAC heard a series of technical and scientific presentations. It also received verbal summaries and accepted written reports from two of its Subcommittees which had met earlier to assess specific areas of PF scientific activity (on Medical Applications and on Electronic Structure). Following questions and discussion, ISAC met in closed session and formulated its observations, conclusions and recommendations. ISAC reached unanimous agreement on the material presented in the closeout to the management of the IMSS and PF held on Wednesday morning, March 5.

This written report summarizes ISAC's findings and recommendations. In the following eight sections are more details and elaboration of the topics in the same order that they were presented in the verbal closeout with IMSS and PF management. The Appendix contains a list of the ISAC members of the Review Committee and the Agenda of the ISAC meeting. Written reports of the two ISAC Subcommittees accepted by ISAC at its meeting are available separately from PF Management.

1. PF, Photon Science and the KEK Roadmap

ISAC considered the PF program in the context of the science institutes and how it maps to forefront and discovery research in Japan and indeed worldwide. ISAC recognizes that PF, the existing Structural Biology Research Center (SBRC), and the proposed Structure Materials Science Research Center (SMRC) within IMSS develop advanced instrumentation and technologies *and* do forefront and pioneering research in strategically selected areas of materials and life sciences. ISAC feels that it is essential that the impact of this research and its importance to Japan be recognized by KEK as a key part of its mission and that the strategic importance of photon science at KEK be an integral and aggressive part of the future roadmap plan for KEK.

The strong motivation for the strategic importance of photon science is illustrated well by considering the domain of the "nanoscale" and the growing importance of discoveries on this scale to enable future progress in areas central to the grand challenges facing energy, environment and biomedical research. The properties of x-rays (including their short wavelength and penetrating ability) greatly enable and drive discovery on the nanoscale – they tell us about where the atoms are and how the electrons behave. X-rays provide the means to understand the basic structure and functionality of materials from the viewpoint of basic science (areas include condensed matter, biological systems, environmental and chemical sciences and many others).

ISAC believes strongly that with vision and planning, KEK can build upon its already

formidable strength in Photon Science (with PF, SBRC, SMRC and the complementary JPARC program) to become among the world's leading laboratories in research that will enable solving some of the most important societal challenges of our time, including the design of new drugs to cure and control human disease and improve our health, understanding of man-made and natural pollution and remediation processes in our environment, development of improved processes and materials underlying clean, efficient, sustainable and environmentally friendly energy production, storage and conversion and understanding, tailoring and controlling the properties of nanostructured materials engineered on the atom scale for advanced technology applications.

2. KEK as a World Leading Center For Scientific Discovery using Photons, Neutrons and Muons

PF and IMSS have developed a vision for the future that is based on two complementary x-ray sources at the KEK main campus: *i*) the existing electron storage rings PF and PF-AR which produce x-rays that are typically referred to as "synchrotron radiation" and *ii)* the planned x-ray Energy Recovery Linac (ERL). The PF provides a well understood, robust and mature means to deliver x-rays that are used for obtaining detailed information on the fundamental interactions between the electrons, spins and atoms in soft and hard condensed matter. This paradigm is driving fundamental investigations across a range of biological and physical sciences. An improved understanding of these interactions is central to progress in many of the "grand scientific challenges" in areas of societal importance.

The ERL is a completely new class of next generation x-ray source. PF and KEK have the remarkable opportunity to build the world's first hard x-ray ERL. ERL x-rays will provide a clear "vision" into systems on the atomic and nanoscale through novel imaging techniques (including systems under extreme conditions of pressure/temperature). Also possible will be the study of systems undergoing real-time reaction and change.

It is very important to recognize that KEK also provides forefront sources for neutrons and muons with the new J-PARC facility. These tools can provide information that is complementary to that obtained with x-rays. While J-PARC is not in the purview of ISAC, we do wish to recognize the unique opportunities that will come from synergy and planning between these facilities. The science institutes provide one of the bridges to enable this to be done and are a key additional element in delivering world class science from the accelerator based facilities at KEK.

Based upon knowledge gained at its first and second meetings, ISAC wishes to emphasize the broad and deep impact of the research done at PF. This impact is strongly facilitated and enabled by the PF accelerator-based light sources and talented scientific and technical staff. PF operates within the environment of KEK which provides a unique and world class environment for accelerator science and excellence for development of current and future generation photon sources.

ISAC appreciates the unique role played by PF within the context of Japanese synchrotron science and urges that KEK recognize this. We especially note that PF provides unique instruments of the highest quality for soft x-ray research in Japan where there has traditionally been world leadership in this important area for condensed matter studies and

atomic and molecular physics. PF and PF-AR continue to be central elements of a successful near-to-medium term strategy for synchrotron science in Japan. The future ERL promises to be a unique, x-ray source complementary to XFEL at Spring-8. The ERL offers a visionary and strategic path for the evolution of on-site, world-leading capabilities. KEK and PF have the responsibility and stewardship of a very important large National and International photon science user community. Currently PF serves about 3000 users from a broad range of scientific disciplines in academia, national laboratories and industry and this number continues to grow. With further enhancements in operations of PF and PF-AR, careful planning, focused R&D and evolution of the PF/PF-AR activities to an ERL, the future is indeed remarkably bright for photon science at KEK.

3. Structure Materials Science Research Center (SMRC)

ISAC recognizes the strategic importance of a focused center that is organized around the study of advanced materials. It is an area that is important for future growth of PF and provides strong opportunities for university/industry ties. ISAC believes that is important to carefully consider the organizational structure that would be most effective to achieve selected scientific goals. We encourage that the PF management broaden the discussion to the wider outside community and rapidly convene a group of experts to visit and advise IMSS/PF on details so that a set of strategic goals can be identified and chosen for the initial phase of SMRC.

ISAC believes that the SMRC can be modeled after the very successful SBRC. Management needs to make a concerted effort to inform and engage staff and outside scientists in the concept for the proposed Center. Important elements also include attracting external funding and cooperation with the user community. ISAC strongly emphasizes that a critical and indeed unique opportunity exists to appoint a world-leading scientist to head the new Center. This position is critical to the strategy of developing photon science as an increasingly strong component of KEK.

The concept for photon science at KEK is very broad (photons, neutrons and muons) and this is unique if developed in a coordinated way. It is also clear that overall strength can be gained by engaging SPring-8 in collaborative ways with the new Center.

4. Areas of Excellence and Beam Line Program

ISAC strongly endorses the strategy and process to identify and focus on areas of excellence. PF Management is strongly encouraged to refine and focus within each of the areas on instruments and opportunities which can be world class and which have a strong underpinning of infrastructure at PF and in the region (including manpower). ISAC is pleased to see the strong progress in the prioritization and relocation/decommissioning of the bending magnet beam lines. ISAC feels that the process has been reasonably aggressive given the complexity of the task (solving the hybrid problem) and providing state-of-the-art soft x-ray IDs. Engagement of the user community seems to have been the case up to now. It is very important that this process continues to be open and managed in close cooperation with the user community.

ISAC urges that in making choices of beam line/instrument reconfiguration decisions, consideration be given as to how best to support the identified areas of excellence. We recognize that the VUV/SX capabilities have been improved and feel that an appropriate fraction of available resources have been assigned for this important restructuring.

With regard to international collaborations, ISAC supports a phased shutdown of BL20B assuming that the instrumentation and support can be maintained at a level where users can obtain excellent access and data. ISAC also continues to support enthusiastically the Indian BL effort. However, it is important to better articulate and quantify the arrangements and understand how this will be mutually beneficial to both parties. This includes plans for budget and manpower for building and operating the BL.

ISAC continues to be concerned about the overall number of beam line scientists being too small to provide optimal performance of the instruments and scientific program of PF. Such performance is absolutely dependent on the number and quality of beam line scientists and thus this number needs to be increased. ISAC urges that PF work with KEK management to develop and support a strategy that will attract and retain more scientists of the highest quality. This is especially important as PF begins to position itself to take stronger advantage of the scientific opportunities that will come from an x-ray ERL.

5. ERL Project

ISAC continues to most strongly support the ERL development in that it offers a route to next generation performance for a Japanese x-ray light source and even more broadly in the world. An ERL compliments the scientific portfolio enabled by SPring-8, XFELs and the other Japanese light sources. Further, it is clear that the important strong engagement of the KEK accelerator division is ongoing and is a key to positioning KEK to be at the forefront of future light source development.

Developing a compelling science case for the ERL project and facility, including organizing and involving the user community, should continue to be a very high priority. We note for example the upcoming science case workshop as a very positive step. PF and KEK are strongly encouraged to continue in this direction.

PF and KEK are urged to Identify commonality among the future accelerator projects at KEK and better integrate and include the ERL (and PF) R&D (and eventually construction) in this core accelerator technologies program. Significant progress in design and critical R&D has been observed by ISAC and PF and KEK are to be strongly complimented and encouraged. For example, the PF/KEK ERL team has demonstrated much progress in the development of the SRF cavity. Presented results on the performance of one cell cavity are the state-of-the art in Q-values and suppression of HOM. The next step in the testing of the 9-cell cavity is critical for the demonstration of integrated technology. ISAC recommends that it is important for the viability of the 5-GeV ERL to establish and achieve well-defined technical specifications for the SRF cavity to be used at the compact ERL.

ISAC applauds the renaming of the “test facility” to the Compact ERL and redefining of the technical objectives and science case. This project is a very important “stepping stone” to the x-ray ERL and we urge that it be constructed with sufficient energy (several hundred MeV) and current (100 mA) to fully demonstrate the principles and operation that are required for mitigating risk in building a high energy x-ray ERL. In order to claim in the future

that the prototype is “a success” it is important to keep as narrow as possible the brackets for such design parameters as emittance.

6. Subcommittee Reports on Medical Applications and Electronic Structure

Medical Applications. The Medical Applications Subcommittee chaired by Prof. K. Shinohara met February 29, 2008, at the Photon Factory, Tsukuba. The report of the Subcommittee is available separately from PF Management. The ISAC received a summary presentation at its meeting from the Subcommittee Chairperson. Following discussion in executive session, ISAC accepted the report and endorsed its conclusions and recommendations. From our perspective in regards the overall IVCAG program, ISAC does not see medical imaging as a key area of excellence at PF and it should not be a focus of significant core PF effort. On the other hand, if external funding for a microangiography end station is forthcoming from the biomedical research community, than such a development could have significant merit and return important scientific discovery in the area of human health. Funding should not come from the PF core budget for this activity. ISAC would welcome the opportunity to hear more about the microtomography program as it evolves and progress is made toward identifying funding sources for a successful venture.

Electronic Structure. The Electronic Structure Subcommittee chaired by I. Lindau met February 27 & 28, 2008, at the Photon Factory, Tsukuba. The report of the Subcommittee is available separately from PF Management. The ISAC received a summary presentation at its meeting from the Subcommittee Chairperson. Following discussion, ISAC accepted the report and endorsed the conclusions that are spelled out in points 1 through 8 of the report.

7. Other Conclusions and Comments

ISAC believes that theory is an increasingly important aspect of progress in many of the science focus areas, especially as the complexity of the problems being addressed grows very large. PF should strategically look to use opportunities for in house appointments and collaboration with outside theory groups to form strategic alliances that bring strong theory components to the selected areas of excellence.

Single bunch operation – It was clear that the fraction of single bunch time should be assigned on the basis of scientific excellence. ISAC does recognize that PF offers unique scientific capabilities in this area. The performance of experiments carried out during this time should be carefully examined and benchmarked.

Other regarding PF accelerators – ISAC compliments the PF accelerator team for the successful demonstration of the capability of top-up operation. Although full implementation of this capability would bring some strain on the injector performance it will nevertheless significantly benefit PF users. The Implementation of the fast polarization switching at the BL-16A will definitely bring new unique capabilities to PF users. The idea of the controlled secondary source for the double IDs sounds very interesting but requires more detailed analysis on the effect of systematic errors introduced by such an optical scheme.

Educational beam line – in principal this is a good idea but it will require careful preparation and could consume significant resources. Impact on PF resources is of concern. PF is in a

unique position to collaborate with outside universities and this is an appropriate direction. PF has been and remains a very important resource for graduate and postgraduate education and training – developing the next generation of scientists.

J-PARC – ISAC recognizes the world-class facilities for neutron and muon research that will be coming on line in the very near future as the J-PARC enters its fully operations phase. We noted earlier in this report the unique opportunities for synergy in targeted research areas between the main campus KEK photon resources and those at JPARC with neutrons and muons. KEK is encouraged as appropriate to facilitate sharing of information between the ISAC and the comparable advisory committee for J-PARC, especially noting the opportunities with using photons and neutrons in synergy to tackle complex problems. Exchange of reports and communication between the chairpersons of the committees are examples of means to achieve this goal.

ISAC was especially pleased with the level and quality of the science presentations. However, the talks could be more focused and shorter. ISAC would like to applaud the PF Director and senior management for its strong leadership and vision during this past year. We thank the PF and outside staff for their excellent science and technical presentations and openness in discussion. Also we thank the administrative staff for their outstanding organizational help and for the very fine hospitality in making our visit very comfortable and efficient.

8. PF ISAC – Processes and Recommendations

Experience of ISAC members with other advisory bodies suggests that a 3-year cycle is most effective. We suggest that membership should rotate on a staggered basis with two 3-year terms for each member being the norm. This longer period of time is especially important for continuity if the goal of 2 meetings per year is not met on average.

ISAC strongly supports the formation of the Review Subcommittees and expresses its willingness to continue to fully engage in this important process. We feel that the first two Subcommittees were especially effective and thank the chairpersons and the members of the subcommittees for their excellent work. ISAC would like to see the reports, or at least a summary, before its meetings if at all possible to facilitate its consideration of the conclusions and recommendations and better integration of them into its full reports.

ISAC membership – we feel that the committee balance is appropriate and about the right size.

ISAC found that the agenda for this meeting was too dense and rushed and there was insufficient time for discussion (including the need for more executive session time). It is important in future meetings to carefully focus the attention of the Committee on the key set of issues for which PF management seeks advice. The ISAC Chairperson will be willing to work with the PF Director well ahead of the next meeting to identify and prioritize the topics so there will be adequate time for thoughtful and informed discussion and recommendations.

ISAC feels that the next meeting date should be in October or November of 2008 and encourages strongly the PF management to begin to obtain calendars of the committee members very soon and fix a date.

Appendix – Contained in the Appendix to this ISAC Committee Report are the following:

1. List of ISAC members

2. Agenda of the ISAC Meeting – April 3-4, 2007

3. Reports of the two ISAC Subcommittees

- **Electronic Structure, I. Lindau Chairperson**
- **Medical Applications, K. Shinohara Chairperson**

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1. List of the Members of the PF ISAC Committee

Ernest Fontes – Cornell High Energy Synchrotron Source
Hidetoshi Fukuyama – Tokyo University of Science
Efim Gluskin – Advance Photon Source
Keith Hodgson – Stanford University, Chairperson of Committee
Ingolf Lindau – Stanford University
Kunio Miki – Kyoto University
Toshiaki Ohta – Ritsumeikan University
M. Ree – Pohang Accelerator Laboratory
Volker Saile – University of Karlsruhe
Hiroyoshi Suematsu – Riken Harima Institute

2. Agenda of the 1st ISAC Committee Meeting

First PF ISAC Meeting

Date: April 3 – 4, 2007

Place: Room 244, Building No.4, KEK

PROGRAM

Tuesday April 3, 2007

9:00-9:10 Introduction and charge to the committee (O. Shimomura & K.O. Hodgson)

9:10-9:30 Photon Factory update (S. Wakatsuki)

9:30-11:10 Response to the PF External Review held in March 2006 (S. Wakatsuki)

Report on the preparation process of the strategic plan (S. Wakatsuki)

The new group structure (S. Wakatsuki)

New schemes for communication with user community and the PF Users Organization (S. Wakatsuki)

Organization of ISAC subcommittees and the next ISAC sometime later in FY2007 (S. Wakatsuki)

11:10-11:30 Coffee break

11:30-12:30 BL strategy and the new beam lines (PF-BL17A, BL3A, BL16A, PF-AR NW14A, NW10A, a pharma BL) and consolidation of BLs (M. Nomura)

12:30-13:30 Lunch

13:30-15:00 Science topics

100-picosecond resolved X-ray studies at the beam line NW14A (S. Adachi PF)

Symmetry breaking and interatomic resonant Auger decay in molecular inner-shell photoionization (A. Yagishita PF)

Structural study of oribital-ordered magnetite thin film (H. Wakabayashi PF)

Structural basis for knock-in-lock dynamics of RNA polymerization (O. Nureki, Tokyo Inst. Tech.)

15:00-15:20 Coffee break

15:20-16:20 Present status of ERL project at KEK (H. Kawata)

Present status of ERL project –Light Source- (T. Kasuga)

16:20-17:00 Discussion with PF directorate (closed session)

17:00-18:00 Executive session (closed session)

Wednesday April 4, 2007

09:00-10:00 Executive session (closed session)

10:00-10:30 Summary discussion