SPring-8学術国際評価委員会（SPARC 2008）報告

独立行政法人理化学研究所
財団法人高輝度光科学研究センター
ＳＰＡＲＣ実行委員会事務局

大型放射光施設SPring-8は、1997年に供用を開始して以来、様々な活動に広く利用されており、2008年秋には創設11周年を迎えた。この間、施設の運営全般に関する評価等、様々な国際評価を受けてきたところであるが、今般、主として学術を中心に、SPring-8の利用成果について国際的レビュアーの評価を受け、施設の果たした意義、役割を検証するとともに、今後の施設運営、利用促進業務の展開への参考とするため、SPring-8学術国際評価委員会（SPring-8 Academic Review Committee、略称SPARC）を、平成20年11月17日～19日の３日間、SPring-8において開催し、同評価委員会による評価を受けた。評価委員にご就任いただいた方々（リスト中、敬称略）は次のとおりである。

[委員会メンバー]

委 員 長　福山　秀敏（東京理科大学、教授）
副委員長　Gerhard Materlik (Diamond Light Source, CEO)
委　　員　Chi-Chang Kao (NSLS, BNL, Chair)
委　　員　Janos Kirz (Advanced Light Source, Scientific Advisor)
委　　員　Sine Larsen (ESRF, Director of Research)
委　　員　Dennis M. Mills (APS, Argonne National Laboratory, Deputy Director)
委　　員　Claude Lecomte (Nancy University, Director)
委　　員　Judith A. K. Howard (Durham University, Head of Department)
委　　員　So Iwata (Imperial College London, David Blow Chair of Biophysics)
委　　員　太田　俊明（立命館大学、教授）
委　　員　藤井　保彦（日本原子力研究開発機構、部門長）
委　　員　鈴木　謙爾（東北大学、名誉教授）

また、同評価委員会のプログラム（概略）は次のとおりであった。

November 16 (Sunday)

20:00　Brief Meeting (Closed)

November 17 (Monday)

08:00　Breakfast Meeting
09:00　Welcome Address (Dr. Akira Kira)
09:10　Opening Remarks (Prof. Hidetoshi Fukuyama)
09:20　General Introduction (Dr. Hideo Ohno)
10:00　SPring-8's Impacts on Synchrotron Radiation Instrumentation (Dr.Tetsuya Ishikawa)
11:00　Structural Biology at SPring-8 (Dr.Takashi Kumasaka)
11:40　Model to Real Target: Lipid Structural Biology as an Applied Science (Dr.Masashi Miyano)
12:05　Structure of a Biological Macromolecular Nanomachine, the Bacterial Flagellum (Prof. Katsumi Imada)
14:10　Imaging and Diffraction Studies in Medical and Biological Sciences (Dr.Naoto Yagi)
14:50　Structural Chemistry in Synchrotron Radiation Science & Technology (Dr.Masaki Takata)
15:30　Chemistry of Nanoporous Materials (Prof. Susumu Kitagawa)
16:20　In-Situ Time-Resolved Dynamic Surface Events on the Pt/C Cathode in a Fuel Cell under the Operating Conditions (Prof.Yasuhiro Iwasawa)
16:45　Soft X-ray Photochemistry at BL27SU (Prof. Kiyoshi Ueda)
17:10　Discussion

November 18 (Tuesday)

09:00　Structural Materials Science Research (Dr. Masaki Takata)
09:40　Structural Studies by Powder Diffraction at SPring-8 (Prof.Eiji Nishibori)
10:05　Structure Science of Strongly-Correlated Electron Systems (Prof.Takahisa Arima)

10:30 Recent Progress in Polymer Science at SPring-8 (Prof.Atsushi Takahara)
11:15 Spectroscopy for Investigating Properties and Functions in Materials Science (Dr.Junichiro Mizuki)
11:55 High Resolution Inelastic X-ray Scattering (Dr.Alfred Baron)
13:40 Electronic Structure of Soft Materials Studied by Soft X-ray Emission Spectroscopy (Dr.Shik Shin)
14:05 Magnetic Materials (Dr.Motohiro Suzuki)
14:30 Recent Advances in Earth and Planetary Sciences (Prof.Tetsuo Irifune)
15:10 Environmental Studies at SPring-8 (Prof.Yoshio Takahashi)
15:50 Industrial Research at SPring-8 (Dr.Yoshio Watanabe)
16:50 Discussion and Drafting
20:30 Discussion and Drafting (cont'd)

November 19 (Wednesday)

09:00 Discussion and Drafting (cont'd)
14:15 Brief Review Announcement (Prof.Hidetoshi Fukuyama)
14:45 Reciprocal Address (Mr.Nobuo Fujishima)
15:00 Adjourn

同評価委員会から提示された報告書の概要（ここでは、スペースの関係上Executive summaryのみ掲載）を以下に掲げる。
（※報告書の全文については、SPring-8のホームページ（http://www.spring8.or.jp/ja/support/）をご覧下さい。）

SPring-8学術国際評価委員会（SPARC2008）

会議報告
開催日：2008年11月17日～19日
場所：SPring-8　上坪講堂

Executive summary

The results of the assessment of the scientific achievements made by SPARC are presented first, followed by the general recommendations.

[A] ***Outstanding achievements***

**** In-vacuum Undulator Sources***

By placing the magnet structure inside the vacuum chamber, the undulator gap can be reduced, and hence much shorter magnetic periods can be built without compromising the strength of the magnetic field. This extends the energy-range of undulators at SPring-8 and all other light sources. The brilliant success of this approach has been leading the way for other facilities and for new sources with medium size accelerators which nowadays even operate at smaller emittance than the first 3 facilities, APS, ESRF and SPring-8. It is also worth pointing out that this concept promises presently a cost saving option for future XFEL sources. Clearly, this development has had a profound worldwide impact.

****Advanced Beamline Technology***

From the start the SPring-8 beamline team has tried to develop new beamline concepts using the source properties in the most optimised way. This has led not only to new designs of monochromators and polarisers, but also to new measurement strategies such as a 1km beamline, modulation spectroscopies and several more.

**** Structural Studies on Membrane Proteins***

It is known that up to 30% of human proteins are located in the cell membrane. These membrane proteins play crucial roles in many biological functions and are of key importance for medicine. We recognized that research on Ca^{2+}-ATPase, bovine Rhodopsin, bacterial multidrug efflux transporter are truly outstanding and to the highest international standard. High flux X-ray beams at BL41XU and BL44XU were essential for these experiments.

**** Structural Studies on Macromolecular Assemblies***

The study of macromolecular assemblies is a particular challenge for structural biology. The flagellum is a huge molecular complex made of 20 to 30 thousand subunits containing about 30 different proteins. High resolution X-ray structures of flagellar component proteins were solved using the brilliant X-ray beams at BL41XU and

BL44XU. By combining these single crystal X-ray results with the low resolution structures obtained using cryo-EM and X-ray fibre diffraction, the structures of three distinct parts of the flagellum were determined.

Real-time SAXS Analysis of Periodosome

The process of assembly/disassembly of the periodosome (a multimeric complex of Kai proteins) was followed in real time by SAXS experiments at BL45XU, which could indeed verify that this was controlled by the phosphorylation of one of the Kai proteins and provided an overall picture of the periodosome in its different states. This real time elucidation of the circadian clock mechanism by Small Angle X-ray scattering is a unique example of the application of real time SAXS experiments. Other examples include the successful investigation of protein folding.

**** Motion of Potassium Channel revealed by Single Molecule Tracking***

By using a novel technique based on monitoring the movements of a gold nanoparticle attached to the KscA potassium channel and irradiating it with white X-radiation, the motion of the protein could be monitored in real time by following the motions of the diffraction spots from the gold crystal. These experiments showed how the potassium channel upon gating was twisted around the pore and that gating could be prevented by adding an open-channel blocker. Single molecule tracking opens unique opportunities to study molecules in action and this was made possible on BL44B2.

**** Rational Design of Nanoporous Materials with Chemical Functionality***

An impressive range of new metal-organic frameworks (MOFs) and Porous Coordination Polymers (PCPs) compounds exhibiting specific chemical functionalities have been synthesized. These compounds have significant commercial potential as potential gas storage, as well as catalytic, media for clean and renewable energy solutions. This program benefits and interplays synergistically with the world-leading small molecule crystallography program at BL02B2.

**** Probing Bulk States of Correlated Electron Systems by High-Resolution Resonance Photoemission***

At a helical undulator beamline, equipped with a varied line space grating monochromator, high-resolution and high-photon flux soft X-ray beamline was realized at BL25SU. This has been successfully utilized in soft-X-ray resonance photoemission experiments of strongly correlated systems. Thanks to a much longer escape depth, bulk electronic states were observed, which previously had been revealed only weakly with a low photon energy photoemission spectroscopy (PES). These results demonstrate the effectiveness of high energy, high resolution PES for the study of strongly correlated 4f electronic states.

**** Phase Change Mechanism of Rewritable Optical Media***

X-ray diffraction pinpoint measurements at BL40XU demonstrate the interest in time-resolved X-ray diffraction for academic and industrial use. Optical recording on DVD media is due to the amorphous to crystalline phase transition of the $Ge_2Sb_2Te_5$ (GST) and $Ag_{3.5}In_{3.8}Sb_{75.0}Te_{17.7}$ (AIST) materials. A direct measurement of the crystallization processes has been studied on a 0.32 micron surface of the DVD itself at nanosecond time-resolution. Comparison between GST and AIST suggests that crystal growth control may be a key for designing faster phase change materials. The quality of the micro beam is paramount for investigating the ultra fast physics of photo-and thermo-excited phase transitions or chemical reactivity, by time-resolved studies.

**** Post-perovskite Phase of $MgSiO_3$ at 120GPa: Nature of the Mantle-Core Boundary***

Under the high-pressure and high-temperature conditions (125GPa, 2,500K) corresponding to a 2,700km depth at the mantle-core boundary, where the D″ seismic wave velocity discontinuity is observed, the crystal structure of the post-perovskite phase of $MgSiO_3$ was successfully analysed, based on the *in situ* X-ray diffraction measurements at the state-of-the-art high-pressure station BL10XU. This newly-solved crystal structure has a striking high-density layered-structure. This feature can solve successfully long standing mysteries, such as the discontinuous seismic change and the seismic anisotropy in the D″ layer.

**** Advancing the Understanding of Automobile Exhaust Gas Catalysts***

Researchers from Toyota are advancing their understanding of Ceria Zirconia—a 3-Way automotive exhaust catalyst. Extended X-ray absorption fine structure (EXAFS) measurements were made on the Ce K-edge (40.45keV) and Zr K edge (18keV) at BL01B1 and BL16B2 to understand the local structure around these atoms and a clear relationship between the oxygen storage/release capacity of the material and its local structure was determined. Through the end of 2006, over 30 million Toyota vehicles have been fitted with this type of exhaust catalyst. This, and other work, clearly has made an impact on Toyota as they are now in the process of constructing an insertion device beamline (BL33XU) at the SPring-8 facility.

In other work on catalysis, scientists from Daihatsu are using BL14B1 to further their understanding of so-called intelligent catalysts with the goal of developing a more durable exhaust gas catalyst. They found that precious metal ions such as palladium, entered and exited the ceramic crystals repeatedly as if they had" intelligence ", and that the ions did not grow larger in size which can reduce the efficiency of their catalytic activity. This information has allowed Daihatsu to achieve a substantial reduction of palladium in their automotive catalysts.

These two examples clearly demonstrate the fact that the basic research with strong motivation can lead to real break-through in applications. Such efforts should be encouraged more.

**** Interfacial Magnetism between FM / AFM Bilayers in Magnetic Sensor Heads***

It is the goal of many hard disk drive manufacturers to reach a recording density of 1 Tb/in^2. With this increase in density, instabilities in the exchange coupling between the ferromagnetic (FM) / antiferromagnetic (AFM) bilayers have been seen where the magnetization in the ferromagnetic layer has changed unexpectedly. Higher robustness is required in the fidelity of the data on hard drives and so experiments were performed at BL25SU to better understand the mechanism of exchange coupling and the control of magnetic structures at FM / AFM interfaces. Previously the existence of pinned interfacial AFM spins had been reported, but the mechanism that stabilises this process was unclear. This work verified the existence of pinned interfacial spins in the anti-ferromagnetic layer.

[B] ***General Recommendations on Future Plans***

**** Revolutionary Instrumentation Development***

Relying on the development (together with Osaka University) of the Elastic Emission Machining of mirrors to reach atomically smooth surfaces, a microfocus of 48nm×36nm has already been demonstrated on the 1km beamline, with remarkably low stray scatter. Furthermore, focusing to 8nm has been demonstrated in one dimension. This is clearly a remarkable record. Particularly exciting plans were announced to extend this technology to the 1nm level by the use of multilayers. In fact, a Kirkpatrick-Baez microprobe with any spot size in the sub-10nm range will be revolutionary!

**** Compact XFEL***

The use of a thermionic gun followed by several bunch compression stages, a C-band warm linac and micro-undulators as emitters, was considered by many specialists, again similar to the in-vacuum undulator approach in the early 90's, a high risk approach. A prototype was built, which has demonstrated brilliantly the viability of the approach, and is now used as a successful user facility with a 20—25eV FEL. Knowing that the prototype is working, the opportunity to realise a short and cost efficient version of an XFEL has become even higher. There are plans to use the FEL as a pump, to be combined with beams from SPring-8, as a stroboscopic probe of time-evolution. This will be a unique capability. Furthermore, electron bunches from the linac will also be available to be injected into SPring-8 to create capabilities for very short X-ray pulses. This would give additional unique scientific opportunities.

**** Improvement of life-science BL***

More and more complex biological systems will be targeted in the future that will require the use of different synchrotron radiation based techniques, *e.g.* diffraction, small angle scattering and imaging. The combination of techniques in the study of biological systems is already

taking place and it is important that SPring-8 continues to facilitate applications of complementary methods. Structural biology evolves towards the study of more and more complex systems that are characterized by small and poorly diffracting crystals. It is therefore necessary to examine many crystals of the same sample to find the one most suitable for the measurements.

The proposed improvements of the MX beamline complex, that aims at creating a beamline portfolio, with each beamline fulfilling a specific role, seems best suited to meet the demands of structural biology in the future and to keep the macromolecular crystallography at SPring-8 at an internationally competitive level.

**** Theoretical Modeling***

Due to their quality, the experimental results sometimes deserve a more thorough theoretical approach, as for example the pioneering work on myoglobin. Similarly, combined with MEM, systematic use of multipolar analysis of electron density would allow better description of inter-atomic interactions and bonding.

**** High Resolution Inelastic X-ray Scattering***

At BL35XU non-resonant meV resolved Inelastic X-ray Scattering should be developed in the future in order to investigate atomic scale correlations in electronic excitations. This requires the construction of a new beamline which will enable important higher resolution measurements of electronic excitations.

**** Synthesis of Nano-Polycrystalline Diamond: Potential Applications for HPT Experiment***

A nano-polycrystalline diamond, named" HIME-DIA ", was successfully synthesised with a special capability of hardness exceeding diamond and low thermal conductivity, potentially accessible to the center of the earth (364GPa, 5,500K). It will benefit also fields such as material and environmental sciences.