Chapter 2

Overview of the SPring-8 Upgrade Plan

2.1 Motivation for the SPring-8 upgrade

SPring-8 is one of the highest performance light source facilities in the world. Its mission is to support our society by producing a great quantity of important research in various fields such as science, industry and culture. In this section, we address the need for the SPring-8 upgrade.

Today, we enjoy the benefits of a modern society with abundant cultural activities, general security and a healthy lifestyle. Our comfortable life and activities are supported by advanced industries and medical services that have been established through years of accumulation of scientific knowledge. Continued development in science and technology is essential to sustain these benefits and achieve further improvements in the future. First, fundamental scientific research is applied to new technological applications. Then industry develops products to address social problems. After the twenty-first century, there are still many unresolved social and environmental problems, such as energy issues, global warming, and treatment for chronic disease and congenital disorders. Potential solutions are closely related to scientific and technological challenges yet to be resolved. The mission of research facilities is to address these social problems through new scientific inventions or discoveries.

Research using hard X-rays is based on physical and chemical processes at an atomic scale. For materials science, useful capabilities in new functional materials (e.g., high efficiency batteries, ultra-dense magnetic recording media, clean catalysts, and semiconductor memory chips) emerge as a result of the electronic nature of materials at the atomic scale. The key fabrication technology for future functional materials will be based on schemes of a self-organization mechanism for reducing energy consumption. For biological sciences, almost all biological activities, such as energy metabolism, gene maintenance and replication, and inter- and intra-cellular signal transduction proceed through the dynamical transition and collaboration of macromolecules. For example, potential drugs reactions can be understood through the dynamics of protein molecules. Thus, research revealing the structure and the dynamics of materials using hard

X-rays, have played and will continue to play key roles in the fundamental sciences during the next twenty years.

This is where SPring-8 comes into play. As SPring-8 is able to generate X-rays, especially hard X-rays of the highest brilliance, many scientists have come from all over the world in order to explore various kinds of research in key fields. From the viewpoint of users, higher brilliance allows *more precise observation during a shorter data acquisition time of smaller objects at a higher spatial resolution.* However, the reason why SPring-8 has attracted many users is not only because of its capabilities as a light source, such as high brilliance and stability, but also because we have contributed to society in two aspects. First, extensive research in fundamental sciences has been completed. As research outcomes have accumulated over the years, the resulting knowledge base will contribute to society through enabling future technological innovations. Second, a large amount of research executed at SPring-8 targets industrial applications in fields such as electronic devices, drugs, batteries, cosmetics, automobile tires, fibers, and polymers. SPring-8 has proved that synchrotron radiation is a useful tool not only for fundamental science but also for a wide variety of industrial applications. Increasing demands for using SPring-8 come from both scientific and industrial fields.

In order to meet the increasing light source requirements, the whole facility has continuously improved. Now, the available experimental time per user is already exhausted and little space remains for improving the capacity of the facility. On the other hand, a number of light sources have been constructed or upgraded in Asia, Europe, and the U.S., especially during the last ten years. Several of these facilities already exceed or plan to exceed current SPring-8 performance in key parameters.

We strongly recommend an upgrade of SPring-8 for the following reasons. In order to support a growing number of users and maintain competitiveness with their research requires improving the light source performance. The upgrade would benefit users from two perspectives. First, the upgrade aims to significantly improve the quality of light (as discussed in detail in the following sections) providing great new capabilities for cutting-edge research. Second, improved light source performance would provide additional opportunities for research by reducing the time required for each experiment. As will be shown, the brilliance of the newly designed facility is 1,000 times greater. It follows that acquisition time would be reduced by orders of magnitude, and with appropriate infrastructure development, more users would benefit from the new light source. Thus, all the research from cutting-edge sciences to industrial works could take advantage of the upgrade. In summary, we conclude that the upgrade of SPring-8 would benefit society by enabling profound new discoveries and technological innovations.

In the following sections, we first state the key concepts of our upgrade plan, also known as SPring-8 II, which provide a platform for world-leading research to be conducted in SPring-8 over the next twenty years. We then briefly introduce the pioneering science research that would be achievable using the upgraded SPring-8. We then close the chapter by showing the superiority of our upgraded facility over other present and planned light source facilities.

2.2 Key concepts of the upgrade

In this section, we present the following key concepts for our upgrade plan and show how these concepts apply to future research:

1. An ultimate storage ring in hard X-ray regime.

2. Synergetic use with the X-ray Free Electron Laser.

3. An energy-efficient facility.

The following sections describe the details of each key concept.

2.2.1 Ultimate storage ring

The first and most important key concept for the upgrade is an ultimate storage ring in the hard X-ray region. We propose to upgrade SPring-8 to "ultimate" status by pushing the light source performance to its limits in two aspects, spatial coherence and brilliance. In the following sections, we present the vastly improved light source performance anticipated by upgrading SPring-8.

Diffraction limit

For the first goal of the ultimate ring, we plan to make the electron beam emittance comparable to the diffraction limit of X-rays so that the spatial coherence approaches unity. The degree of spatial coherence is determined by a product of the beam size and the divergence, known as photon emittance. In a storage ring, a circulating electron beam emits light. Its emittance is calculated from a combination of the electron beam emittance (defined in the same way as that of the photons it produces) and the photon emittance contributed by a single electron. Thus, as the electron emittance decreases, the photon emittance of light generated from a storage ring improves (i.e., decreases), and correspondingly the spatial coherence of light improves. However, the photon emittance has a minimum attainable value due to the diffraction properties of light. The intrinsic minimum product is called the diffraction limit, and is written as $\sigma_r = \lambda/4\pi$. For $\lambda = 0.1$ nm, for example, the diffraction limit is $\sigma_r \approx 10$ pm.rad. In the upgrade program, we propose to make the electron beam emittance in the same order as the diffraction limit, σ_r. The current electron emittance of SPring-8 is 3,400 pm.rad. We propose to reduce it by about

100 times with the upgrade to SPring-8 II, which would result in a dramatic improvement in the spatial coherence of the light.

Using an X-ray beam with such a large spatial coherence length would provide users with new opportunities for focusing experiments with nanometer-order probe beams. Moreover, the scanning coherent X-ray imaging (ptychography) method [1–3] would become much easier for users with orders of magnitude shorter acquisition time and for objects with various sizes. All these methods, not accessible in other facilities, would enable SPring-8 to complete world-leading research and to study more complex, smaller structures in materials that are important in various fields of science. In other words, the upgraded facility would be best suited to solve the hierarchy within various systems as summarized in Sections 2.3.1 and 3.1.

Ultimate brilliance

For the second goal of the ultimate ring, we plan to achieve ultimate brilliance from a storage ring. For this purpose, the huge improvement in electron beam emittance mentioned above works well. The reduction of emittance by a couple of orders of magnitude would bring the brilliance to a significantly higher level than what is currently available at SPring-8. In addition, we will develop insertion devices, especially in-vacuum undulators, in which making shorter undulator periods and narrowing the undulator gap will be key objectives. A combination of the improvement of insertion devices and a great reduction in the emittance of the electron beam is expected to increase the brilliance of SPring-8's light to an ultimately high level. Our plan is to provide high brilliance undulator radiation, in the X-ray region with energies up to 100 keV. Details of the accelerator development and the resulting spectra of light are presented in Chapters 5 and 6, respectively.

A great improvement in the brilliance practically enhances opportunities of experiments and effectively increases beamtime by a factor of around 1,000. This results in two important effects. First, it leads to a remarkable increase in the number of acceptable users. Second, it results in a significantly larger number of measurable samples per beamtime due to the shortening of the acquisition time. The latter effect will lead to a new statistical analysis using a synchrotron radiation source for the first time (see Sections 2.3.2 and 3.2).

2.2.2 Synergetic use with the X-ray Free Electron Laser, SACLA

The second key concept is to develop a facility where unique science and technology concepts are tested by using both SPring-8 II and SACLA, the new X-ray free-electron Laser (XFEL) facility. First, SPring-8 will have the option of using the XFEL linac as an injector for the newly designed storage ring (as discussed in detail in Section 5.2). This is advantageous because the new injector, having extremely low emittance beams, matches well with the new storage ring, and it is also cost effective. The new injector provides very short electron bunches, which may also benefit the short X-ray pulse generation in the storage ring. Second, construction of the XFEL-SPring-8 experimental facility was completed in 2011. In this facility, an experimental hutch was built where the same sample can be illuminated by X-ray beams from both SPring-8 II and SACLA. Many frontiers of science cultivated by the synergetic use of these two light sources are surveyed and summarized in Section 2.3.3 and Chapter 4.

2.2.3 Energy-efficient facility

The third key concept of the upgrade of SPring-8 is to design an energy-efficient facility. As mentioned in Chapter 1, the upgrade plan aims not only to significantly improve the light source performance, but also to make it energy-efficient. First, we will fully utilize existing resources such as buildings and equipment. Although it imposes several major constraints on the new accelerator design as discussed in Chapter 5,the reuse of as many resources as possible is regarded as one of the most important bottom line benefits in the upgrade plan. Second, a new storage ring will be designed such that it consumes less energy than the current ring. Energy efficiency is a growing concern for current and future scientific projects. The newly designed light source will match the demand for a more sustainable society by yielding orders of magnitude higher performance with less energy consumption. As discussed in Chapter 5, the newly designed storage ring would reduce energy consumption by about 30 %, or even much more if we opted for an alternate design (see Table 5.8).The light brilliance generated by the new ring is estimated to be 1,000 times higher (see Fig. 6.1), and the increase of the flux at a sample could become even larger as indicated in Chapter 6. Thus, the upgrade plan proposes a considerably more energy-efficient facility.

Our strategy of reconstructing beamlines is to yield the best quality and highest brilliance beams at a maximum number of beamlines. In terms of beamline optical axes, we will keep the optical axes of normal undulator beamlines fixed, while bending beamline optical axes may eventually be moved by the new accelerator design. Additionally, plans call for mini-undulators with a short period (total length 10 cm) which generate a higher brilliance of X-rays than the existing standard undulators, due to the extremely low electron beam emittance.

2.3 Pioneering science using the upgraded SPring-8

In this section we show the expected benefits and the breakthrough in various fields of science using the new technologies achievable with the upgrade plan, which could never be achieved with the current SPring-8 configuration.

2.3.1 Resolving the hierarchy within systems using diffraction limited X-rays

The first new target in science for the next 20 years will be to clarify the hierarchical arrangement and its temporal evolution within systems that have spatial and temporal in-homogeneity. For such observations, SPring-8 II's beam would be a particularly effective tool, with its high brilliance, its high spatial coherence and its short time duration.

A diffraction limited hard X-ray beam could be achieved on the millimeter scale at SPring-8 II where the majority of X-rays are spatially coherent due to the extremely small emittance of the source in two dimensions (see details in Section 6.1). In Coherent Diffraction Imaging (CDI), a lens-less microscopy technique, an electron density distribution of an object in real space is retrieved from its recorded X-ray diffraction patterns. The observation of objects with a wide range of sizes, between millimeters and sub-micrometers, would be possible by scanning CDI (ptychography) method [1–3] for achieving a large field of view. The structural hierarchy of various biological and material samples could be elucidated for the first time using X-ray imaging as the main tool. CDI measurements are also planned at XFEL facilities, where hard X-rays with a slightly better spatial coherence are expected to be generated. However, an extremely high photon number within a short pulse duration, on the order of 10 fs, causes severe radiation damage to nearly all samples exposed. SPring-8 II would be the most powerful tool for elucidating the hierarchical organization within scientific objects using such ultimate, non-destructive imaging, since such research cannot be performed at existing XFEL facilities. The scientific outcomes expected from the research on these structural hierarchies is summarized in Section 3.1.

2.3.2 Statistical analysis using intense brilliance of X-rays

The second major target for science over the next 20 years will be to resolve the fundamental nature of individual differences using statistical analysis. For such a study, often more than 100 measurements are needed over the samples grown in the same conditions. The best way of obtaining statistically significant data over such a large number of samples would be to prepare samples with a very small size, which matches the focus size of the high intensity focused X-ray beam. SPring-8 II would provide an ideal beam for such experiments because the high degree of spatial coherence (see Section 6.1.5) enables diffraction-limited focusing and more than four orders of magnitude higher X-ray intensity to 50 nm focus size, compared with existing SPring-8 capabilities (see Section 6.3.3). More than four orders of magnitude higher throughput would completely change the conceptualization of the measurement schemes using synchrotron radiation (SR). Only well-characterized specimens, in terms of composition and so on, have been processed in conventional SR applications due to the long measuring times for each specimen to obtain statistically significant data. SPring-8 II would remedy this problem. A new methodology using statistical analyses would clarify the fundamentally fluctuating nature of specimens. Namely, statistical analysis using SR measurements would be truly effective in science for the first time. This new approach would be especially powerful for research identifying local atmospheric environments by analyzing the nano-particles within the atmosphere, or in cell imaging to clarify the specific properties of specimens that are usually hidden by natural variations. This breakthrough due to the radical increase of the brilliance of SPring-8 II and the statistical analysis it facilitates is summarized in Section 3.2.

2.3.3 New Sciences enabled by two ultimate light sources

Aside from the previous two scientific targets, the upgraded SPring-8 engenders unique scientific capabilities arising from the synergy and complementary use with SACLA, the X-ray Free Electron Laser (XFEL). The construction of SACLA was completed in the 2010 fiscal year and its commissioning was successfully carried out in the 2011 fiscal year. Combined with the neighboring SACLA, SPring-8 II would be a unique ring source at which samples can be illuminated by the two different types of X-ray sources.

These two sources are complementary and can be used in a synergetic way as explained below. The X-ray beam from SACLA is characterized by extremely high peak brilliance, a billion times higher than that of SPring-8, a short pulse width, on the order of 10 fs and high spatial coherence. This source is attractive for many applications, e.g., allowing the fundamental processes of atomic movements to be elucidated on a femto-second time scale. On the other hand, the radiation damage to samples would, in most cases, be much less severe using SPring-8 II due to the much reduced peak brilliance, several orders of magnitudes lower than SACLA, although the brilliance averaged over time of SPring-8 II would be orders of magnitude larger. Moreover, the high repetition rate of approximately 100 MHz enables observations on a wide time scale, ranging from pico-seconds to minutes. Therefore, non-destructive measurements, especially for material sciences research, and the temporal evolution of various systems could only be effectively performed by SPring-8 II. The complementary use of SPring-8 II and SACLA (correlative imaging) would enable the observation of a wide field of view and a localized area of the same sample. The synergetic use of these two sources would enable the elucidation of the coherent optical processes in the X-ray region. The prospects for these new sciences are summarized in Chapter 4.

2.4 Status of Other Light Source Facilities

SPring-8 was constructed as one of three large third generation synchrotron radiation sources, together with the European Synchrotron Radiation Facility (ESRF, France/EU, 1995) and the

Advanced Photon Source (APS, USA, 1996). SPring-8 user operations started in 1997. The facility has provided a high brilliance X-ray beam and contributed to various breakthroughs in photon sciences by national and international researchers. Since 2000, medium sized, high quality rings have been constructed at various sites around the world. Two new projects under construction, the NSLS-II in the USA and the MAX-IV in Sweden, plan to exceed the emittance of the three large facilities, although the targeted X-ray ranges of the two new light sources are not exactly the same as those of the three facilities. Meanwhile, the 6-GeV light source, PETRA-III of DESY, began operations in 2009. The emittance of the PETRA-III reaches 1 nm.rad, smaller than SPring-8 and others, and now there are four large synchrotron radiation sources in the world. On the other hand, developments of XFELs, the fourth generation light source, are progressing in Japan (Hyogo, SACLA), USA (Stanford, LCLS) and Europe (Germany, Euro-FEL & FLASH). Additionally, compact FELs in the ultra-violet and soft X-ray regions are being developed at various sites around the world. To summarize, several sources having superior beam quality compared with SPring-8 and having completely different beam characteristics will be operational within the next ten years. The evolution of these sources has made a marked difference in both the quantity and quality of information obtained from experiments, as witnessed by the rapid development of X-ray and visible light sciences after the inventions of synchrotron radiation sources and lasers. Without doubt, the performance capabilities of the source are closely linked to the scientific achievements possible in the future. For our nation to maintain our stance in the forefront of science and technology, we need to lead in the development of synchrotron radiation sources. The purpose of the upgrade program is to maintain SPring-8's position as a center of excellence, leading the field of photon sciences during the next 10 to 20 years, only possible with innovative improvements in the accelerator and the light source quality. After this upgrade, SPring-8 II would have no equal in light-source performance. The diffraction-limited source in the hard X-ray region, in principle, would presumably have the highest performance in terms of brilliance. There are currently no definite proposals at other facilities for similar diffraction-limited sources in the hard X-ray region. The high brilliance in the hard X-ray region, one of the major merits of the large storage ring, would be maintained after the upgrade, giving SPring-8 II a significant advantage over medium size ring sources.

2.5 Contents of the report

In the following chapters, the results of various investigations for the upgrade of SPring-8 are presented. In Chapter 3, the scientific goals to be achieved during the next 10 to 20 years are listed. In Chapter 4, the pioneering areas of science that require the synergistic use of SPring-8 and SACLA are outlined. In Chapter 5, the list of technologies and the R&D required for the accelerator components are summarized. Chapter 6presents estimates for the improved properties of the source and the X-ray beam at the sample position in an upgraded SPring-8. This report summarizes the discussions about the upgrade program that occurred during the fiscal years of 2008 and 2010 within our working group. In Appendix, the history of the activities of the working group is summarized. The names of participants in the working group and the committee members for the upgrade of SPring-8, belonging to RIKEN (Institute for Physical and Chemical Research), JASRI (JApan Synchrotron Radiation research Institute), Osaka University and International Medical Center of Japan, are listed before Chapter 1 of this report. This report will be published as the proposal from the SPring-8 facility as of 2011. We are grateful for any opinions or proposals from national or international researchers for further improvements to our proposal.

References

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