White Paper

and

Activity Report

RIKEN SPring-8 Center Advisory Council 2011

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Message from the RSC Director

This document, "White Paper and Activity Report for RSAC 2011", covers the activities of the RIKEN SPring-8 Center (RSC) since the previous RSAC in February 2009, which was three years after the first RSAC in February 2006. In the 2009 RSAC, we asked the advisors to assess the mission-oriented reforms of the RSC's reorganization into three divisions: Innovative Light Sources, Photon Science Research and Advanced Photon Technology. In parallel, we reviewed the status of the XFEL construction project. Some problems with the organization had already been pointed out during RSAC 2009, though the RSC had only recently restructured into the three divisions. Although we did not immediately respond to the suggestions, we took the suggestions seriously and continued to make changes. In particular, various proposals were made regarding the management of the XFEL facility after its completion, partly because it was not very clear at that time which entity would ultimately be responsible for XFEL management. We consider the management issue to be not wholly within the RSC, but heavily related to the RIKEN Harima Institute. Even so, we temporarily set up a fourth division, XFEL Research and Development, in the RSC to manage the XFEL facility.

One of the serious challenges facing the RSC is generational change. Dr. Hideo Kitamura, head of the Coherent Synchrotron Light Source Physics Laboratory, left the Chief Scientist position in March 2009 and moved to the XFEL Project Head Office as the director of the Insertion Device Development Group. Dr. Masashi Miyano, head of the Structural Biophysics Laboratory, moved to Aoyama Gakuin University in Tokyo as a professor, keeping a temporary visiting Chief Scientist position at the RSC. The recruitment process for the new Chief Scientists is currently operated jointly with the RIKEN Nishina Center (RNC) and the Advanced Science Institute (ASI), both located in the RIKEN Wako Institute. This process is worth consideration without excluding possible alternatives.

In 2009, the screening process to reduce the national budget reviewed the management process of SPring-8. This proved momentous for the RSC, although the RSC was not directly involved in SPring-8's management; rather the relationship between the RIKEN Harima Institute was examined to suggest improvements. The overall conclusion was that RIKEN and JASRI had to make the management of SPring-8 more effective and transparent. To accomplish this, the RIKEN Harima Institute should redefine its management roles and responsibilities for SPring-8, and possibly, for the new XFEL facility.

Construction of the XFEL facility was going smoothly. Soon after the previous RSAC 2009, construction of all the buildings completed. Installation of the accelerator completed in March 2011 followed by commissioning of the electron beam. Soon after, we observed spontaneous X-rays from undulators at the optics hutch of the photon beam line. The facility was named SPring-8 Angstrom Compact free electron LAser (SACLA). After three-month commissioning, SACLA finally lased at 16:10 on June 7, 2011, with a wavelength of 1.2 Angstroms, followed by progressive shifting towards shorter wavelength.

Returning to the SPring-8 SR facility, we are happy to announce that the four long straight sections in the storage ring have all been allocated to beam lines. One of them is the inelastic scattering beam line, BL43LXU, to be built by the RSC. The RSC has constructed another challenging beam line, BL32XU, for macromolecular crystallography with a micro-focused beam. We have started discussions on the next upgrade of the SPring-8 ring, with a goal of completion during the 2019 fiscal year.

In this booklet we give a brief introduction and recent activities of the RSC. We will present additional information not included here at the meeting in July 2011. We hope that these materials help provide an idea about the overall activities of the RSC and that the Advisory Council will provide us with valuable comments and advice regarding management of the RSC going forward.

June 2011

Tetsuya Ishikawa
Director, RSC

Chapter Ⅰ

The RIKEN SPring-8 Center

- The Leading Photon Science Research Complex -

Chapter 1 The RIKEN SPring-8 Center
- The Leading Photon Science Research Complex -

1. Organization Consolidation toward Goal-Oriented Management

Photon Science using Synchrotron Radiation (SR) has increasingly contributed to progress in a wide range of Science and Technology all over the world. To meet the ever-increasing demands for SR applications, quite a few countries have been vigorously promoting SR facilities and related science. In Japan, RIKEN and the Japan Atomic Energy Research Institute (JAERI) completed construction of SPring-8, the world brightest SR facility, in 1997. SPring-8 had a dual function: the Japan Synchrotron Radiation Institute (JASRI, see APPENDIX I), entrusted by RIKEN, oversaw public use, while the RIKEN Harima Institute (see APPENDIX II), a branch of RIKEN, performed leading photon science research.

The withdrawal of JAERI from SPring-8 management in 2005 persuaded RIKEN to establish the RIKEN SPring-8 Center (RSC) to ensure that the research institute would remain the World's Photon Science Center of Excellence (COE). The RSC aimed to make the Spring-8 facility the internationally leading institute for synchrotron radiation (SR) science with the following missions:

i. to explore, promote and lead research utilizing unique and advanced SR related facilities at the SPring-8 site,
ii. to upgrade SPring-8 and develop next generation SR sources, and
iii. to contribute to increasing recognition for SPring-8 and to apply its research results in advanced uses of the SPring-8 facility.

The RIKEN Harima Institute has persistently performed general management and administrative functions. As a consequence, the RSC has successfully made further advances in SR through a string of innovations in technologies for accelerator, insertion device and X-ray optics. This progress in Photon Science resulted in assembly of a Compact SASE Source and led to the promotion of the unique X-ray Free Electron Laser (XFEL) project. Construction on the XFEL started in 2006 and completed March 2011. The new XFEL facility named "SACLA" (SPring-8 Angstrom Compact free electron Laser) produced the first laser light on June 7th. In response to the 1st RSAC2006 and 2nd RSAC2009 recommendations, the RSC introduced a mission-oriented organization structure (Fig.1). Among the changes, after RSAC2009, the XFEL Research and Development Division was launched as the newest division. The RIKEN Harima Institute has now two Photon Science facilities: SPring-8, the SR facility, and SACLA, the XFEL facility. The RSC is responsible for facility upgrades and future plans for SPring-8 and SACLA. Now that SACLA is operational, the RSC has a 4th mission:

iv. to facilitate XFEL science emerging from SACLA.

The RSC oversees the following four divisions:

1. Innovative Light Sources Division - responsible for the technical development of advanced synchrotron radiation (SR) sources (including SACLA) and the upgrade of existing light sources (including SPring-8).

2. Photon Science Research Division - responsible for promoting scientific research made possible with innovative light sources. The Division carries out cutting edge research in vast fields of life science, materials science and physical science at the SPring-8 site and is seeking to open new interdisciplinary scientific fields by developing innovative analytical tools.

3. Advanced Photon Technology Division - responsible for the development of measurement technologies to make the best use of the SPring-8 and the SACLA facilities. The Division is developing both hardware and software that will enhance the usability of innovative light sources, thus providing easier access to outside users, including industrial sectors.

4. XFEL Research and Development Division - responsible for conducting and synthesizing research and development of XFEL science from accelerator technology to beam application research (such as ultrafast science) at SACLA. The Division will also establish next-gen photon science by promoting synergies between SPring-8 and SACLA.

In order to maintain its standing as the World's Photon Science Center of Excellence, the RSC has cultivated a cooperative relationship among these four divisions to achieve the four missions. The RSC is also carrying out cross-sectional reviews of the research groups to further align their individual goals toward the RSC missions. In 2010, Dr. Ryoji Noyori, the President of RIKEN, presented the new RIKEN policy as moving "from ST (Science and Technology) to STI (Science, Technology and Innovation)". Consistent with the recent "Noyori Initiative", the RSC upgraded RIKEN's problem-solving leadership in basic and applied research for Photon Science. As a second generation Leading Photon Science Research Complex that will direct SACLA in addition to SPring-8, the RSC is expected to improve both facilities.

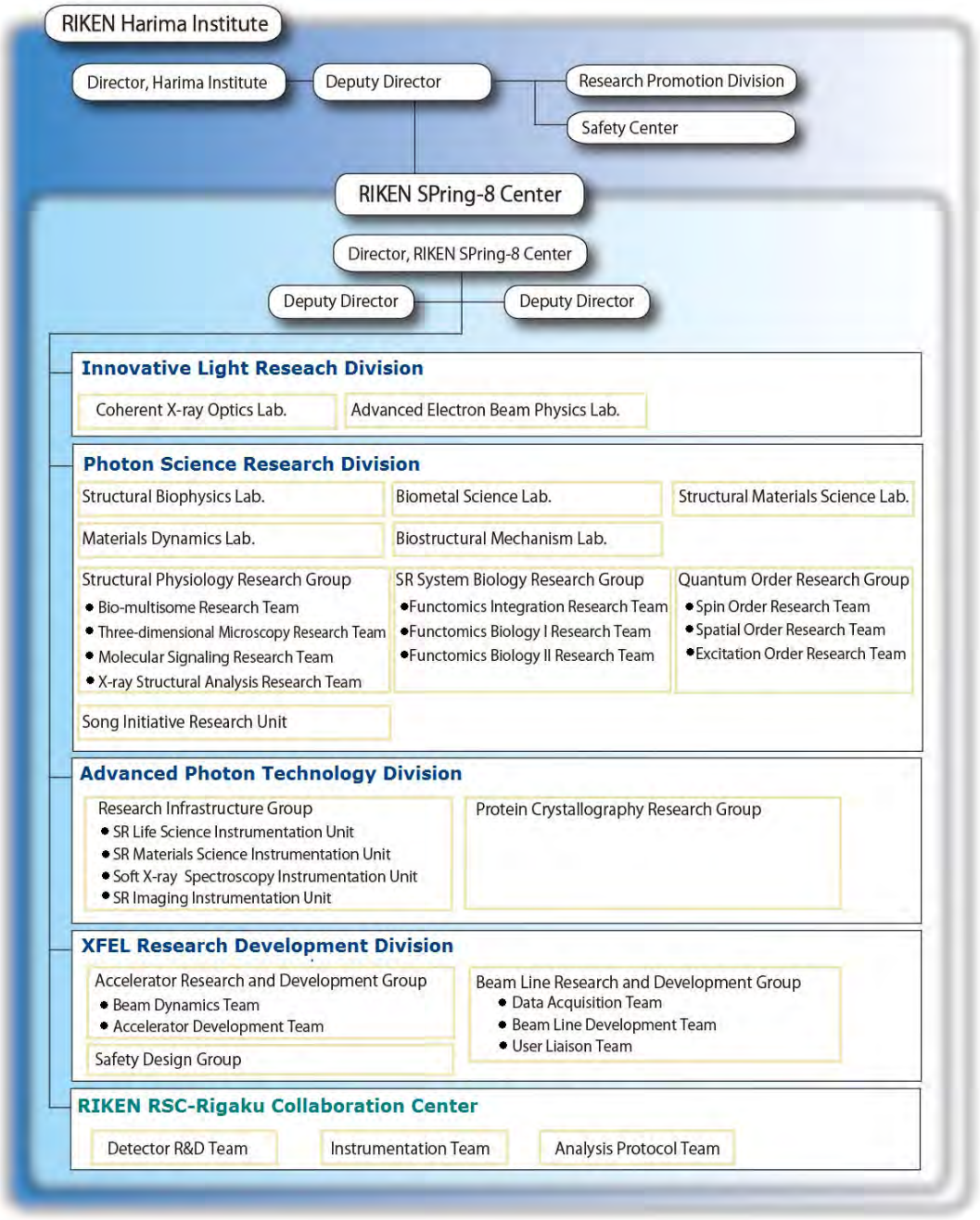


Fig. 1 Organizational Structure of the RIKEN SPring-8 Center

2. Deployment of the State-of-the-Art XFEL (SACLA)

The RSC has confirmed the XFEL laser oscillation in June 2011 and will commence user operations in the latter half of the 2011 fiscal year. Building construction was completed in May 2010. The RSC's XFEL facility, named "SACLA", will be the world's second X-ray Free Electron Laser (XFEL) facility, following the successful inauguration of the LCLS facility at the SLAC National Accelerator Laboratory in the US.

SACLA is the first XFEL facility originally designed for Photon Science Research. Since 2000, Dr. Tetsuya Ishikawa has planned and organized the XFEL project with cooperative research and development at SPring-8. Of particular note is the compactness of the SACLA facility. Its reduced size was achieved by integrating many pioneering innovations developed by Drs. Hideo Kitamura, Tsumoru Shintake and Tetsuya Ishikawa of the Innovative Light Sources Division. The facility utilizes key technologies adopted from SPring-8, such as in-vacuum undulators and ultra-high performance X-ray optics. SACLA has another unique benefit when compared with LCLS and Euro-XFEL. Its location adjacent to the SPring-8 storage ring will afford unique capabilities such as synergistic applications of SR and XFEL and special operation of the SPring-8 storage ring by electron bunches injected from the SACLA linac. Consequently, the deployment of SACLA will open the door to the second stage of the RSC as the headquarters for an advanced Photon Science Research Complex (Fig.2). Therefore, further efficient coordination of SACLA and the SPring-8 accelerator (such as a common control system) may be required for continued scientific research as well as operational cost savings.

Fig. 2 The SPring-8 /SACLA Photon Science Research Complex

There is no doubt that SACLA and the use of intense, coherent, short-pulse X-ray will lead to breakthroughs in Photon Science and change the foundational framework of many scientific fields, including the following:

- atomic, molecular and cluster phenomena
- plasma physics
- condensed matter physics
- materials science
- ultra-fast chemistry
- life-sciences, structural biology
- quantum optics and non-linear processes

Indeed, striking results from pilot research using the SCSS test accelerator machine (250MeV) and RIKEN beam lines at SPring-8 have stimulated many promising ideas for SACLA utilization. The number of applications from around the world submitted for access to the test machine has increased each year. The XFEL Research and Development Division therefore has the challenging task of leading the scientific applications unique to SACLA as well as cross-coupling utilization with SPring-8. In order to maximize the SACLA/SPring-8 synergetic diversity of Science and Technology applications, the Photon Science Research Division and the Advanced Photon Technology Division should also be at the vanguard of innovative change for photon science through cooperative activity with the XFEL Research and Development Division in the RSC's future planning. The organization of the XFEL user community is also critical to launch SACLA, the state-of-the-art XFEL, to a promising start.

3. Research Activities of the RIKEN SPring-8 Center

The research strategies of the RSC were developed with consideration of the recommendations of RSAC2009 (see APPENDIX III for more details). The general areas of focus for research activities are illustrated in this section, while those of the individual groups are presented in Chapter 3 of this white paper.

3-1. Innovative Light Sources Division

The mission of the Innovative Light Sources Division is "the technical development of advanced synchrotron radiation (SR) sources and X-ray FEL and the upgrade of existing light sources at SPring-8". In the last few years, a top priority has been completing construction of the XFEL/SPring-8 equipment, which started in 2006 and finished March 31, 2011. The Advanced Electron Beam Physics Laboratory and the Coherent X-ray Optics Laboratory joined with the XFEL/SPring-8 project to play an important role. We contributed to technology development and

installed the following key devices: (1) a low emittance electron source, where we use a single crystal thermionic cathode and a velocity bunching system (originally developed by the RSC), (2) a high gradient C-band accelerator system to drive the e-beam up to 8 GeV, and (3) an in-vacuum short-period undulator. In addition to RSC contributions, scientists from JASRI participated in the development of the XFEL/SPring-8 facility. We are pleased to report that the project progressed as scheduled and completed construction as planned in March 2011. We started beam commissioning last February, and found machine performance to surpass the required X-ray FEL specifications. After three-month commissioning, we observed successfully the first lasing at 1.2 Å on June 7th. Effort towards lasing at the shorter wavelength is ongoing as exemplified by the fact that it took only three days to reach next milestone of 1.0 Å lasing on June 10th.

We will continue to upgrade the XFEL/SPring-8 facility. We plan to improve coherency by introducing seeding technology at X-ray wavelengths, and to achieve higher flux by using the multiple bunch operation scheme. At the same time, we will continue to develop accelerator technologies required for the SPring-8 upgrade, including beam diagnostic tools, stable girders for focusing elements, high performance accelerating cavities, and stable power supplies. Since there are many common scientific issues and technologies regarding electron linear accelerators and storage rings, the knowledge accumulated in XFEL/SPring-8 will prove useful in upgrading the SPring-8 storage ring.

3-2. Photon Science Research Division

As described in the RSAC2009 recommendations, the overall mission of the Photon Science Research Division is “carrying out cutting edge research in life science, materials science and physical science at SPring-8”. In order to provide the RSC the potential to become a truly world leading center, the RSC received the following recommendations for Life Science and Materials Science:

(Life Science)

Appointment of a proper coordinator with the responsibilities:

i. to promote closer interactions among the research teams, and
ii. to ensure the continued development and optimal use of research infrastructure and resources.

(Materials Science)

Investigation of research opportunities related to energy and the environment with a focused, cross-cutting approach.

To address the recommendations on Life Science, the RSC invited two PIs to join our division in 2009. Dr. Changyong Song moved from the RIKEN Wako Institute as an Initiative Research Scientist. He established the Song Initiative Research Unit and developed research activities focused

on “coherent X-ray diffraction tomography” and “FEL single-shot diffractive imaging”. His research activity covers broad-based targets from biological systems to functional nanomaterials by developing an imaging methodology with coherent X-rays. His participation has also improved the methodological research potential for 3D structural imaging via SPring-8, Electron Microscopy as well as XFEL. During the last three years, he organized three International Workshops on FEL Science and expanded the XFEL science community network. Dr. Yoshitaka Bessho moved from the RIKEN Yokohama Institute as a Team Leader of Functomics Biology II Research Team to focus on the system biology on enzymes and the bio-molecular imaging method for XFEL. The commencement of SACLA operations will enhance dynamic, cohesive interactions among researchers and may improve coordination of research activities for structural biology as well as materials science.

In response to the recommendations on Materials Science, the research groups were further strengthened by new collaborations with the Tokura FIRST Project (Funding Program for World-Leading Innovation R&D on Science & Technology, 2009-2013) by Prof. Yoshiki Tokura (University of Tokyo, RIKEN) and the CMC project (Center of Materials Crystallography, The Danish National Research Foundation, 2010-2014) by Prof. Bo Iversen (Aarhus University). Both projects are aiming to develop a new approach for designing functional materials relating to energy and environment issues (superconducting, spintronics, catalysis, thermoelectric materials, energy storage, etc.) in Physics (Tokura-FIRST) and Chemistry (Iversen-CMC). The laboratory-based collaborations with Prof. Takuzo Aida (University of Tokyo, RIKEN), Prof. Hideo Hosono (Tokyo Institute of Technology, Hosono-FIRST) are also conducive to the materials science relating to functional polymer brushes, organic electronics, electro-conductive cement, iron-based superconductors, etc. Prof. Susumu Kitagawa (Team Leader, Space Order Team) has improved the direction of “green chemistry” with his ERATO and NEDO projects. The successes from these collaborations were achieved by using X-ray Diffraction, Magnetic Scattering, Spectroscopy and Small Angle Scattering with the beam line support of the Advanced Photon Technology Division and JASRI. Some joint programs with the XFEL project are being designed with the XFEL Research and Development Division and the Advanced Photon Technology Division.

Finally, it should be noted that the start of the new RIKEN inelastic X-ray scattering (IXS) beam line (RIKEN Quantum Nano Dynamics Beamline: BL43LXU) will open new research opportunities for investigation of electronic excitations in the eV energy loss regime and cause an impact on structural dynamics research with the complementary use of other IXS beam lines (BL35XU:JASRI and BL11XU:JAEA).

3-3. Advanced Photon Technology Division

The Advanced Photon Technology Division is responsible for the development of measurement

technologies to make the best use of SPring-8 synchrotron radiation and the XFEL. The division is developing both instrumentation and methodologies at SPring-8 beamlines and experimental facilities at RSC which will enhance the performance and usability of innovative light sources in collaboration with the Innovative Light Sources Division and the Photon Science Research Division, thus providing easier access to outside users, including researchers from industrial sectors.

RIKEN has been operating seven characteristic beamlines and has been constructing two front-end beamlines as pilot beamlines in order to facilitate research and development of the instrumentation and measurement technologies at SPring-8. The scientific fields and measurement methods covered by RIKEN beamlines have expanded widely from life science to materials science and physics, and from diffraction and scattering to spectroscopic analysis and imaging.

The division is composed of two groups: the Research Infrastructure Group and the Protein Crystallography Research Group.

The Research Infrastructure Group is in charge of RIKEN's beamlines. The Research Infrastructure Group formed in November 2008 with two units: the SR Life Science Instrumentation Unit and the SR Materials Science Instrumentation Unit. In response to the expansion and deepening of RIKEN's SR scientific research, the group added two more units. The Soft X-ray Spectroscopy Instrumentation Unit was launched in February 2010 and the SR Imaging Instrumentation Unit was formed in April 2010. These units focus on enhancing and promoting research and development for the beamline technologies for soft X-ray spectroscopy and X-ray imaging, respectively.

The SR Life Science Instrumentation Unit has continued and enhanced support of structural biology research to operate RIKEN Structural Genomics BL26B1 & B2 and opened the door for protein micro-crystallography by constructing a new beamline: the RIKEN targeted protein BL32XU with 1-micron focused X-rays.

The SR Materials Science Instrumentation Unit established the new research fields of pico-seconds time-resolved X-ray diffraction with pump-probe technique and space-resolved X-ray magnetic scattering with 100nm focusing optics at RIKEN SR physics BL19LXU. By using the time-resolved X-ray diffraction system equipped with a synchronized femto-second pulsed laser, we observed laser-induced lattice deformation and acoustic pulses in semiconductor wafers. BL44B2 was switched to a materials science beamline, named RIKEN materials science, to tackle the precise analysis of exotic nanomaterials.

The Soft X-ray Spectroscopy Instrumentation Unit is in charge of the development, improvement and generalization of various spectroscopic tools as well as cutting-edge utilization technologies for soft X-ray (SX) spectroscopy based on RIKEN Coherent Soft X-ray Spectroscopy BL17SU. As a unique experiment, high-resolution soft X-ray photoelectron spectra of liquid water (H2O and D2O) were successfully measured at BL17SU. It was found that the experimental results were consistent with the conventional model of a tetrahedral hydrogen network in liquid water.

The SR Imaging Instrumentation Unit is responsible for infrastructure development for various X-ray imaging and for evaluation of XFEL instruments. The development of cutting edge X-ray imaging techniques, such as coherent diffraction microscopy and nano-focusing, as well as hard X-ray photo-electron spectroscopy, paves the way for outstanding achievements in the medical, biological and material science fields. The Osaka University group broke the 10 nm barrier for X-ray beam width and succeeded in forming 7 nm X-ray beams at BL29XUL for the first time in the world. BL29XUL and BL19LXU are also utilized for R&D for XFEL instrumentation and experimental techniques as platforms for ultra-fast time resolution and coherent imaging, respectively.

The Protein Crystallography Research Group develops various elemental technologies for protein crystal engineering, including a novel protein crystallization method using micro-porous zeolite, and improves automatic systems of protein crystal growth and supporting software for structure analysis. Through those developments, the group constructs high-throughput frameworks to resolve hard analytic protein structures. The group also operates the Protein Tectonics Platform (PTP) at RSC. The PTP enables beamline users to conduct efficient and complete protein science experiments within the SPring-8 campus. The PTP is now released to various research groups inside and outside RIKEN.

4. Global Assistance as a Pivotal Photon Science Center

The RSC has designed various global cooperative programs to develop a multi-disciplinary and comprehensive strategy for the multilateral promotion of Photon Science. The roll-out of these programs has expanded the international SR facility network and provided valuable feedback on a variety of levels of SR science and technology. In Photon Science, major upgrades are underway at existing world class SR facilities (ESRF, APS, PETRAIII) and new SR facilities have opened or will open shortly in Switzerland, France, England, Australia, Canada, China, Taiwan and Sweden. All three XFEL facilities, LCLS, SACLA and Euro-XFEL will be operational within 10 years. The impact of all these new facilities on science will be immense. The RSC, as the leading research and development entity in RIKEN Harima Institute owning SPring-8 and SACLA, assumes global responsibility for conducting international collaborative program to develop a mutually complementary relationship between the SR institutes and scientific communities (see APPENDIX I).

4-1. International SR/XFEL Workshops with SR/XFEL Institutes

In addition to the Three-Party Meeting, which is the collaborative workshop for the European Synchrotron Radiation Facility (ESRF), the Super Photon Ring-8 GeV (SPring-8), and the Advanced Photon Source (APS), the RSC has organized subject-oriented workshops on SR science with the SR

institutes based on the cooperative MOU agreement on SR science and technology. The SR institutes involved are APS (USA), BNL (USA), ESRF (EC), SLAC (USA), DESY (GE), ALS (USA), PAL (ROK), PSI (CH), NSRRC (Taiwan), SLRI (Thailand), Australian Synchrotron and KEK (Japan). The workshops have addressed a wide range of subjects including Accelerator R&D, X-ray Optics, Nanoscience Applications, and XFEL science. The workshops have energized exchanges of SR technology among the facilities and provided support to improve progress in technologies such as accelerator, insertion device, X-ray optics, measurement control, detector system, and SR applications.

A Neo-Three-Party Meeting of the RSC, DESY and SLAC has also been organized to improve the quality of individual XFEL projects by promoting the exchange of information from the latest R&D in XFEL science. The RSC has organized several regional XFEL meetings, including Asia-Oceania international workshops on FEL science in Korea (Feb. 2009), Taiwan (Dec. 2009) and Japan (Oct. 2010). The workshops inspired intense discussions of XFEL applications among leading scientists from Japan, Korea, Taiwan, Australia, and the US and facilitated the promotion of XFEL projects in the region.

The RSC has also provided strong support for the Asia-Oceania Forum of Synchrotron Radiation Research (AOFSRR). The AOFSRR was established in 2006 as a regional network organization to promote collaboration and cooperation among the member facilities and user communities in the Asia-Oceania region for the development of synchrotron science and technology. The principal activities are the AOFSRR workshops (Japan: 2006, Taiwan: 2007, Australia: 2008, China: 2009, Korea: 2010) and the Cheiron School (SPring-8), which is the annual school teaching comprehensive synchrotron science and technology for junior scientists and engineers in the Asia Oceania region since 2007(Fig.3). The RSC will continue to support AOFSRR integration and extension toward the Pacific Rim.

Fig.3 The Cheiron School

4-2. Collaborative Research Programs

The RSC is conducting several collaborative research programs as the key institute. In 2009, the RSC started scientific collaboration with POSTECH in Korea, expanding the existing cooperation on the SR facility between the Pohang Accelerator Laboratory (PAL), the RIKEN Harima Institute, and JASRI. Several POSTECH professors have frequently visited RIKEN beamlines to conduct new research. Workshops have been held with various topics, including “Applications of XFEL”, and more are being planned. The RSC has offered beamtime on RIKEN beamlines in addition to the general public beamlines to PLS users during the recent shutdown of the Pohang Light Source (PLS).

In 2010, the Center for Materials Crystallography (CMC) project of Aarhus University in Denmark was initiated to establish a world-leading center to address key challenges in materials science such as unraveling the chemical origin of molecular self-assembly, measuring excited state crystal structures, and obtaining atomic scale insights into complex magnetic materials. An important aspect of this application-oriented project is to form a research network including both the large SR facilities (SPring-8: RSC, APS: ChemMarCARS) and the Neutron facility (SNS: Oak Ridge National Laboratory). The RSC is one of the key members of this project and is exchanging scientists and PhD students to conduct SR experiments.

Collaboration with the Max Plank Institute (MPI, Germany) is proceeding under the global RIKEN-MPI collaboration agreement, covering detector development for XFEL and application of XFELs in the atomic, molecular and optical (AMO) field. Joint experiments have been carried out by using the SCSS test accelerator.

A long-standing Daresbury-RIKEN collaboration has grown into the University of Liverpool (UoL, UK)-RSC collaboration because a UK representative moved from Daresbury to UoL. Collaboration on structural biology using both SPring-8 and SACLA is underway. RIKEN and the UoL commenced a Joint Graduate School program in which the RSC accepted a PhD student from UoL. In addition, collaboration with the National Synchrotron Radiation Center (Thailand) and other institutes is in the planning stage.

New collaborative programs for coherent X-ray science have recently been organized with The Gwangju Institute of Science and Technology (GIST) / The Center for Extreme Light Applications (CELA) in Korea, The Indian Institute of Science (IISc), and The ARC Centre of Excellence in Coherent X-ray Science (CXS) in Australia. The XFEL research network will further extend its reach, increasing the number of such collaborative programs.

The RSC established the Protein Tectonics Platform (PTP) in 2007 to maintain the activities of the High Throughput Protein Factory (HTPF) after completing the Protein 3000 Project. The RSC started the collaborative program with the NSRCC in Taiwan in 2009 with a mission to enable beamline users to conduct efficient and complete protein science experiments at the SPring-8 site based on utilization of the PTP. The PTP is recognized as a high-performance facility that provides for all aspects of determining the crystal structure of proteins: gene manipulation and expression, purification, characterization, crystallization, in-house diffraction experiments, and crystallographic computations.

4-3. The RIKEN RSC-Rigaku Collaboration Center

It is well known that recent progress in Photon Science relies on a disparate range of elaborate technologies. The RSC recognizes the importance of encouraging activities in engineering development relating to Photon Science with the instrument industry. As a model project, the RIKEN RSC-Rigaku Collaboration Center was established in 2010 (Fig.1) in order to develop technologies to allow a seamless connection of X-ray emission and applications - ranging from laboratory instruments to large-scale synchrotron radiation facilities - or the advancement of structural biology and material science in Japan. The ultimate objective is to provide a research environment for everyone working in these fields, including scientists in industry.

One of the goals of this center is to enhance the high-throughput protein crystal structure analysis technology originally developed for the Protein 3000 Project for a shared-use infrastructure platform. The following specific component targets will be developed:

i. Two-dimensional detectors and data processing
ii. Synchrotron radiation measurement technology for use in the laboratory
iii. New systems for using protein structure analysis

To achieve these targets, the center invited three scientists as team leaders: Drs. Takaki Hatsui (Detector R&D Team), Sono Sasaki (Instrumentation Team) and Naoki Kunishima (Analysis Protocol Team).

4-4. Graduate Programs

The development of both domestic and international human resources is an essential ingredient to the progress of Photon Science. The RSC is conducting an international cooperative program with POSTEC (Pohang University of Science and Technology) and is joining with the RIKEN cooperative program at Liverpool University. The RSC is also extending its network of cooperative graduate programs with several key universities across the nation. To date, thirteen universities including the University of Tokyo and Osaka University have programs promoting Photon Science and Synchrotron/XFEL Research. The RSC has sent more than thirty staff as visiting professors to the universities and provided comprehensive and coordinated educational efforts related to both SPring-8 and SACLA.

5. Towards Innovative Research Enterprise
Including Cross-Cutting National Research Initiatives

As a result of the recommendations of both RSAC2006 and RSAC2009, the RSC organization has improved significantly as a mission-oriented research entity. As a measure of the improvements, the RSC successfully completed construction of two new beamlines: BL28XU (Advanced Basic Science for Battery Innovation, Kyoto University) and BL36XU (Catalytic Reaction Dynamics for Fuel Cells, The University of Electro-Communications) founded by NEDO in cooperation with JASRI in 2010. The Advanced Soft-material Beamline, BL03XU (Advanced Soft-material Beamline Consortium, 19 Industries-Universities Alliance), started operations in April 2010. These three beamlines share operations and management, governed by collaboration with industries and universities. A new model for advanced industrial applications will be created resulting from innovative utilization of these beamlines. As a result, competitive cross-cutting research may eventually promote reorganization of the Academy/Industry user community.

Of national importance was our recent success in upgrading BL37XU and BL39XU to become nano-beamlines for XAFS and X-ray fluorescence analysis by the Research-Network Building Program for Reduction of Carbon-dioxide Emission of the Ministry of Education, Science and Technology. The program aims to integrate research results and knowledge of “green nanotechnology” in order to accelerate applications for environment technology, in particular by forming a goal-oriented research network. In order to achieve innovative research through the fusion of related research fields, eighteen research centers for the research network “Low-Carbon Research

Network (Lcnet)" were created in Japan. In the Lcnet, the RSC was designated as the SR Nano-beam Analysis Center for Green/Nanotechnologies to develop strategies and methods for solving problems for the advancement of Green/Nanotechnologies using a high brilliance X-ray 100nm beam. The center expects to contribute to materials research for a wide range of energy sources, including Lithium batteries, fuel cells, solar devices, and greenhouse technologies.

On March 11, 2011, the Great Tohoku Earthquake severely damaged and shut down some of Japan's major quantum beam research facilities, including PF and J-PARC, which have contributed to cutting-edge research not only in Japan but worldwide. The initiatives of the RSC are expected to preserve the international competitiveness of Japan in science, technology and industrial development and to become an engine for the restoration and/or reconstruction following the worst natural disaster ever faced by Japan. In May, the RSC decided with JASRI to take emergency responsibility for acceptance and support of the user experiments of the PF and J-PARC facilities by establishing the "Priority Program for Disaster-Affected Quantum Beam Facilities".

The SR and the XFEL provide innovative, luminous electromagnetic waves, which serve as powerful probes for visualizing various levels of materials relating to virtually the whole span of research in science and technology. For the RSC's next major challenge, discussions about a major upgrade of SPring-8 are underway, with a proposed completion date in 2019. This initiative is partly based on build-out projections - SPring-8 will be near capacity with fifty-seven beamlines in operation by 2012. The long term nature of this goal means that the RSC will not undertake an immediate stereotypical upgrade based on existing technologies. Instead, the RSC will create an "ultimate schema" of the storage-ring-based light source, to be accomplished after a series of breakthroughs. This upgrade will require more intensive collaboration, both domestically and internationally, in addition to the RSC's partnership with JASRI. The RSC, as the Leading Photon Science Research Complex with SPring-8 and SACLA operating under the RIKEN Harima Institute, will be required to commit to growing its leadership in Photon Science (Fig.4).

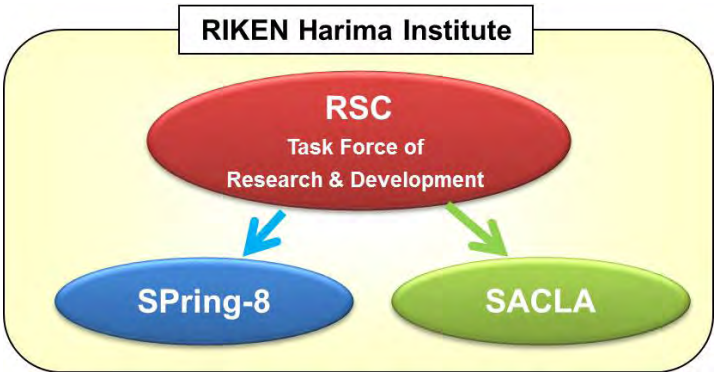


Fig 4. The RIKEN Harima Institute and the RIKEN SPring-8 Center

Consequently, the roles of the RIKEN Harima Institute as the owner of this dual facility complex should be urgently defined to cover all required functions via outsourcing to third parties, except for

those directly entrusted from the government to the registered organizations.

In conclusion, the RSC, equipped with the SPring-8 and SACLA facilities, has entered a new era to blaze a trail for problem-finding and problem-solving oriented science and technology. Therefore, further strengthening of our research and administrative organizations and cooperating systems is one of our primary challenges to remain a leading innovative research enterprise.

Chapter Ⅱ
Terms of References
for The RIKEN SPring-8 Center Advisory Council

Chapter 2 Terms of References for The RIKEN SPring-8 Center Advisory Council

Terms of References for RSAC

The RSAC2011 committee is requested to provide advice specifically on the following topics:

1. a review of improvements to the management system of the RSC (especially its organizational structure and administrative systems) after RSAC2009 with the aim of making the RSC a world-leading Photon Science Research Complex,

2. an evaluation of the research programs and the collaborative activities inside and outside RIKEN that are currently being conducted or are planned for the RSC (from the viewpoints of both scientific and social/societal impacts), and

3. an assessment of the roles that the RSC is expected to take in the research complex with the SPring-8 and SACLA facilities in the Harima site.

Reference

[I] Terms of References for the 8th RAC

1. Evaluate RIKEN's responses to the recommendations made in the 7th RAC report, "RIKEN: Laying the Foundation for Creative Advancement".
2. Under its third 5-year plan from April 2013 to March 2018, RIKEN will continue to pursue its current mission and also use its full resources as a comprehensive scientific research institute to contribute to the gathering of knowledge essential for humanity's continued existence. The 8th RAC is asked to advise on the governance, strategies, research systems, and management policies necessary to achieve this goal.
3. The 8th RAC is asked to evaluate RIKEN's cross-boundary research activities among its Centers and Institutes, as well as its domestic and international collaborative activities with universities, industry, and other external institutions. It is also asked to advise on how to maximize RIKEN's collective strengths.

[II] President Noyori's suggested topics for deliberation by the Advisory Councils for RIKEN's Centers and Institutes

1. Does the Center/Institute have achievements of major scientific significance and/or social impact?

2. Does the Center/Institute have a functioning Plan-Do-Check-Action (PDCA) cycle? In particular, are the mechanisms for reorganizing, improving or closing laboratories working effectively?
3. Are the personnel management practices (hiring and employment conditions) of the Center/Institute appropriate to its world-class standing? Are the quality and the diversity of researchers being maintained at a sufficiently high level? This is a major concern of President Noyori.
4. Evaluate the Center/Institute's collaborative activities within and outside RIKEN, as well as its efforts to promote international collaboration.

Chapter Ⅲ
The RIKEN SPring-8 Center
- Research Activities of Laboratories and Groups -

1. Innovative Light Source Division

1-1. Coherent X-ray Optics Laboratory / 石川 X 線干渉光学研究室

Chief Scientist; Tetsuya ISHIKAWA, Dr. Eng. / 石川 哲也
Since July 1995

A. Research Topics (Highlights)

1. The X-ray Free-electron Laser (XFEL) Project

The laboratory members have joined the construction of the 8-GeV main accelerator, the in-vacuum undulator and the beamline of XFEL. They also collaborate with outside users in R&D of the apparatuses for the initial experiments at XFEL, which are coherent X-ray diffraction microscopes and a femto-second timing system.

2. Optics for Coherent X-rays and Their Applications

Close collaboration with Prof. Yamauchi's group of Osaka University achieved the world smallest 7-nm x-ray beam at 25 keV. Now two-dimensional focusing in a signle nanometer scale is under progress. A scanning fluorescence microscope was reformed to be more famirilar system, and was re-installed in the 1-km beamline for mediacal and biological applications.

Various optical elements for XFEL, such as diamond crystals, beam splitters, and windows, were characterized using highly coherent beam available at the 1-km beamline.

3. X-ray Nonlinear Optics

A new precision diffractmeter for X-ray nonlinear optics was developed, which enabled experimental obervation of parametric down-conversion into the vacuum ultraviolet, the extreme ultraviolet, and the soft X-ray regions. Theoretical understanding of the process was deepened to estimate quantitatively the second order nonlinear susceptibility. Strong resonant enhancement was found for diamonds at the carbon K-edge, for the first time.

4. X-ray Berry Phase Optics

Lateral translation of X-ray beam was observed in a deformed silicon crystal. The observation was agreed quantitatively with the theoretical prediction based on Beryy phase effect. The result opened a new frontier in x-ray optics and fundamental phsics.

5. Coherent X-ray Diffraction Microscopy

The improved microscope makes it possible to measure biological samples without stain. Three-dimensional images were obtained for unstained viruses and human chromosome, that demonstrate the ability of visualizing the inner structure. A coherent X-ray diffraction microsopce combined with a speckle-free focusing system was developed, and used for analyzing the structure of nano-cube with a resolution as fine as 4.2 nm.

6. Applications for Material Science

The performance of hard X-ray photoelectron spectroscopy (HAXPES) has been improved to measure not only core levels but also valence band of new functional materials. Recoil effect of photoelectrons in the Fermi-edge of simple metals was found.

A new ultrahigh vacuum diffractometer was developed for soft X-ray resonant scattering

experiment. The diffractometer was used to observe the electromagnetic structures of strongly correlated electron systems, such as high-T_C superconductors and multiferroic materials. For example, the magnetic chiral domain structure was revealed for helimagnets.

B. Research Subjects

(1) Generation and application of coherent X-rays
(2) High precision X-ray optics and optical instruments
(3) Applications of synchrotron radiation for ultra-fast phenomena

C. Projects

Project name	Category	Started	Completed
Investigation of the relationship between X-ray parametric down-conversion and bond charge	Kakenhi, Grant-in-Aid for Exporatory Research	FY2007	FY2008
Development of a femto-second precision timing delivery and measurement system for XFEL	MEXT, XFEL Research Promotion Program	FY2006	FY2008
Research and Development of Basic Technologies for Visualization of Materials Science Phenomena by Coherent Scattering	MEXT, XFEL Research Promotion Program	FY2007	FY2009
Theoretical and experimental study on X-ray parametric nonlinear processes for application to material science	Kakenhi, Grant-in-Aid for Scientific Research (B)	FY2008	FY2010
Investigation of local optical response using x-ray nonlinear diffraction	JST, PRESTO	FY2009	FY2012
Research and development of optical and control system for X-ray free-electron laser	MEXT, XFEL Research Promotion Program	FY2009	FY2010
Observation of anomalous shift of x-ray wave packet inside crystal nearby Bragg reflection condition and application of the effect to x-ray wave guide	Kakenhi, Grant-in-Aid for Scientific Research (B)	FY2009	FY2013

Recoil effect of Photoelectrons	Kakenhi, Grant-in-Aid for Scientific Research (B)	FY2008	FY2010
Research and Development of Resonant Soft X-ray Diffraction under High Magnetic Field	Kakenhi, Grant-in-Aid for Scientific Research (A)	FY2009	FY2011
Research and Development of Soft X-ray Diffraction for Structural Chirality	Institute Program	FY2008	FY2010

D. Members

as of March 1st, 2011

	number	Name
Research Scientist	14	Tetsuya Ishikawa, Hitoshi Yamaoka, Ashish Chainani, Yasutaka Takata, Kenji Tamasaku, Yoshikazu Tanaka, Toru Hara, Takashi Tanaka, Yoshihito Tanaka, Yoshiki Kohmura, Hisashi Naito, Makina Yabashi, Nobuhiro Go, Kenichiro Tanaka
Technical Scientist	0	
Research Staff	0	
Technical Staff	0	
Visiting Researchers	55	
Trainees	21	

E. Funding

(million yen)

	FY2008	FY2009	FY2010
Laboratory budget from RIKEN	49	16	14
Competitive fund in RIKEN	3	23	0
Competitive fund outside RIKEN	92	36	41
Other fund from University, Private foundations etc.	0	0	0

F. Research Output

	FY2008	FY2009	FY2010
International Publications	34	55	24
Publications in Japanese	3	15	8
Oral Presentations	103	124	91
Patent Applications	0	1	0

a. Papers

(1) Mimura H., Handa S., Kimura T., Yumoto H., Yamakawa D., Yokoyama H., Matsuyama S., Inagaki K., Yamamura K., Sano Y., Tamasaku K., Nishino Y., Yabashi M., Ishikawa T., and Yamauchi K.: “Breaking the 10 nm barrier in hard-X-ray focusing”, Nature Phys. **6**, 122-125 (2010).

(2) Tamasaku K., Sawada K., and Ishikawa T.: “Determining X-ray Nonlinear Susceptibility of Diamond by the Optical Fano Effect”, Phys. Rev. Lett. **103**, 254801-1---254801-4 (2009).

(3) Kohmura Y. , Sawada K., and Ishikawa T.: "Berry-Phase Translation of X rays by a Deformed Crystal", Physical Review Letters **104**, 244801-1--244801-4 (2010)

(4)Nishino Y., Takahashi Y., Imamoto N., Ishikawa T., and Maeshima K.: “Three-Dimentional Visualization of Human Chromosome Using Coherent X-ray Diffraction”, Phys. Rev. Lett. **102**, 018101-1---018101-4 (2009).

(5)Takahashi Y., Zettsu N., Nishino Y., Tsutsumi R., Matsubara E., Ishikawa T., and Yamauchi K.: “Three-Dimensional Electron Density Mapping of Shape-Controlled Nanoparticle by Focused Hard X-ray Diffraction Microscopy”, Nano Lett. 10, 1922-1926 (2010).

(6) Takata Y, Kayanuma Y., Oshima S., Tanaka S., Yabashi M., Tamasaku K., Nishino Y., Matsunami M., Eguchi R., Chainani A., Oura M., Takeuchi T., Senba Y., Ohashi H., Shin S., and Ishikawa T.: "Recoil effect of photoelectrons in the Fermi edge of simple metals ", Phys. Rev. Lett. 101, 137601-1—137601-4 (2008).

(7) Takizawa M., Hotta Y., Susaki T., Ishida Y., Wadati H., Takata Y., Horiba K., Matsunami M., Shin S., Yabashi M., Tamasaku K., Nishino Y., Ishikawa T., Fujimori A., and Hwang H. Y.: "Spectroscopic evidence for competing reconstructions in polar multilayers $LaAlO_3/LaVO_3/LaAlO_3$", Phys. Rev. Lett. 102, 236401-1—236401-4 (2009).

(8) Taguchi M., Chainani A., Matsunami M., Eguchi R., Takata Y., Yabashi M., Tamasaku K., Nishino Y., Ishikawa T., Tsuda S., Watanabe S., Chen C.-T., Senba Y., Ohashi H., Fujiwara K., Nakamura Y., Takagi H., and Shin S.: "Anomalous state sandwiched between Fermi liquid and charge ordered Mott-insulating phases of Ti_4O_7", Phys. Rev. Lett. 104, 106401-1—106401-4 (2010).

(9) Ohtsuki T., Chainani A., Eguchi R., Matsunami M., Takata Y., Taguchi M., Nishino Y., Tamasaku K., Yabashi M., Ishikawa T., Oura M., Senba Y., Ohashi H., and Shin S.: "Role of Ti 3d carriers in mediating the ferromagnetism of Co: TiO_2 anatase thin films ", Phys. Rev. Lett. 106, 047602-1—047602-4 (2010)

(10) Tanaka Y., Takeuchi T., Lovesey S.W., Knight K.S., Chainani A., Takata Y., Oura M., Senba Y., Ohashi H., and Shin, S.: "Right Handed or Left Handed? Forbidden X-Ray Diffraction Reveals Chirality", Phys. Rev. Lett., 100, 145502 (2008).

b. Oral Presentations (* Invited presentation)

(1) Takata Y.: "Hard X-ray Photoelectron Spectroscopy", 11-th International Conference on Electronic Spectroscopy and Structure (ICESS-11), Nara, Japan, October (2009)*

(2) Chainani A.: "Hard X-ray Photoelectron Spectroscopy of Strongly Correlated Electron Systems", International Workshop on Hard X-ray Photoelectron SPectroscopy, Paris, France, January (2010)*

(3) Tamasaku K.: “Recent progress in x-ray nonlinear optics”, Gordon Research Conference X-ray Physics, Waterville, USA, Aug. (2009)*

(4) Tamasaku K.: “Recent progress in X-ray Nonlinear Optics”, 19^{th} International Conference on Laser Spectroscopy ICOLS2009, Hokkaido, Japan, Jun. (2009)*

(5) Tamasaku K.: “Recent progress in x-ray nonlinear optics and future perspectives”, Workshop on Evolution and control of complexity: key experiments using sources of hard x-rays, Argonne, USA, Oct. (2010)*

G. Future Plan

The user operation of XFEL will start in FY2012. In this context, one of the main activities of laboratory should be focused on the innovative use of XFEL. Therefore, the whole laboratory is expected to cooperate to enhance each specialty. Novel X-ray optics, such as X-ray Berry phase optics and X-ray nonlinear optics, will be further investigated not only to understand their fundamental aspects but also to find firm applications with XFEL as well as SPring-8. The well-established technique, such as HAXPES and soft X-ray resonant diffraction, will be extened for time-resolved measurement with XFEL. Coherent X-ray diffraction microscope should be more sophisticated and give new knowledge rather than demonstrations of methodology.

We will present the next-10-year direction of research activity on which the retreat of RIKEN beamlines in SPring-8 will be based. One of the key points is to get a synergistic effect from XFEL and SPring-8. The other is the upgrade of SPring-8. In parallel, the laboratory members should be promoted to outside position in the next few years.

H. Curriculum Vitae (Chief Scientist)

NAME: Tetsuya ISHIKAWA

DATE OF BIRTH: January 12, 1954

EDUCATION:

1977: Graduated from Department of Applied Physics, Faculty of Engineering, The University of Tokyo
1979: Master Degree from Department of Applied Physics, Graduate School of Engineering, The University of Tokyo
1982: Dr. Engineering from Department of Applied Physics, Graduate School of Engineering, The University of Tokyo

DEGREES: Dr. Eng.

APPOINTMENTS:

1982: SPS Fellow
1983: Research Associate,
Instrumentation Division, Photon Factory, KEK
1989: Associate Professor,
Department of Applied Physics, Faculty of Engineering,
The University of Tokyo
1993: Joint Appointment of Visiting Chief Scientist, SPring-8 Project Team, RIKEN
1995: Joint Appointment of Chief Scientist, Microwave Physics Laboratory, RIKEN
1996: Quit the University of Tokyo, adopted as a permanent staff of RIKEN
1997: Chief Scientist,
Coherent X-Ray Optics Laboratory at Harima Institute of RIKEN
Joint Appointment of Optics Group Leader, Beamline Division, JASRI
1998: Joint Appointment of Visiting Professor, Himeji Institute of Technology
2001: Joint Appointment of Deputy Director, Beamline-Technical Division, JASRI
2002: Joint Appointment of Director, Beamline-Technical Division, JASRI
2005: Joint Appointment of Visiting Professor, Hyogo University which is the former Himeji Institute of Technology
2006: Director,
RIKEN SPring-8 Center, RIKEN Harima Institute
Project Leader,
X-ray Free Electron Laser Project Head Office
2010: Director,
RIKEN Harima Institute

ACADEMIC ACTIVITIES:

1992-1993: Councilor, Japanese Society for Synchrotron Radiation Research
1995-1996: Councilor, Japanese Society for Synchrotron Radiation Research
1998-1999: Councilor, Japanese Society for Synchrotron Radiation Research
2001-2002: Councilor, Japanese Society for Synchrotron Radiation Research
2004: Councilor, Japanese Society for Synchrotron Radiation Research
2002: Research Award from the Crystallography Society of Japan
2003: Fellow, SPIE, The International Society for Optical Engineering
2006: Hyogo Science Prize
2007:Science and Technology Prize, commended by the Minister of Education, Culture, Sports, Science, and Technology

1-2. Advanced Electron Beam Physics Laboratory / 新竹電子ビーム光学研究室

Chief Scientist; Tsumoru Shintake, Dr. PhD Engineering/ 新竹　積
Since 2002

A. Research Topics (Highlights)

1. Technical R&D for X-ray FEL

In order to realize Free Electron Lasers at X-ray wavelength, we need certain technologies on the low emittance source, the stable accelerator, reliable beam diagnostics and precise undulator. Under SCSS project, our laboratory has developed (1) low emittance electron source base on single crystal CeB6 thermionic cathode, (2) velocity bunching system, (3) high gradient C-band accelerator and (4) cavity-type beam position monitor (RF-BPM). The undulator for FEL was developed by Prof. Hideo Kitamura and his group.

2. XFEL/SPring-8 (SACLA) construction

All member from our group jointed to construction project of XFEL/SPring-8. K. Togawa contributed to electron source and injector part, T. Inagaki constributed to construct 8 GeV main accelerator (S-band and C-band systems). Y. Otake and H. Maesaka developed stable rf and timing distribution system, beam diagnostic instruments (BPM, OTR profile-monitor, toroid, streak camera system, and rf-deflector cavity).

B. Research Subjects

(1) Low emittance electron source development.
(2) High gradient C-band accelerator development.
(3) High precision beam diagnostic system development.

C. Projects

None

D. Members

as of March 1st, 2011

	number	Name
Research Scientist	5	Tsumoru Shintake, Yuji Otake, Kazuaki Togawa, Hirokazu Maesaka, Takahiro Inagaki
Technical Scientist	0	
Research Staff	0	
Technical Staff	0	
Visiting Researchers	0	
Trainees	0	

E. Funding

(million yen)

	FY2008	FY2009	FY2010
Laboratory budget from RIKEN	7	6	11
Competitive fund in RIKEN	0	0	0
Competitive fund outside RIKEN	0	0	0
Other fund from University, Private foundations etc.	0	0	0

F. Research Output*

	FY2008	FY2009	FY2010
International Publications	6	3	0
Publications in Japanese	0	1	0
Oral Presentations	17	11	13
Patent Applications	2	3	0

*****As a member of XFEL project

a. Papers

(1) Shintake T., Tanaka Hitoshi, Hara T. and Tanaka Takashi et. al., "A compact free-electron laser for generating coherent radiation in the extreme ultraviolet region", Nature photonics, 555, Vol. 2 (2008)
(2) Shintake T. and XFEL/SPring-8 Joint Team, “Status Report on Japanese XFEL Construction Project at SPring-8”, proc. IPAC’10, Kyoto, Japan (2010)
(3) Togawa K., Shintake T., Inagaki T., Onoe K., Tanaka Takashi, Baba H., and Matsumoto H. “CeB6 Electron Gun for Low Emittance Injector”, Phys. Rev. ST Accel. Beams 10, 020703 (2007)
(4) Shintake T. and SCSS Team, “Fist Lasing at SCSS”, proc. FEL2006, Berlin, Germany (2006)

b. Oral Presentations (* Invited presentation)

(1) Shintake T.:”Status Report on Japanese XFEL Construction Project at SPring-8”, IPAC’10, Kyoto, Japan, May (2010)*
(2) Inagaki T.: “8 GeV C-band Accelerator Construction for XFEL/SPring-8”, LINAC’08, Victoria, British Columbia, Canada, Sept. (2008)*
(3) Otake Y. :”Development Status of Beam-Monitor System at XFEL/SPring-8 (Its remporal resolution issue)”, LINAC’08, Victoria, British Columbia, Canada, Sept. (2008)

G. Future Plan

Our laboratory will contribute to SACLA on the following ascpect.

(1) There are several hardware problems remained in SACLA main accelerator. We need to carefully correct and improve them.
  (a) Need to improve reliability of klystron power supply, especially the inverter type PFN capacitor charger, HV feeder cable, and pulse transformer. All of causes are

known, thus corrections will be straightforward.

(b) Fluctuation of AC-line directly affects the heater power of thyratrons and klystrons. AC line has to be stabilized.

(c) 400 V AC-line drives PFN capacitor charger. The circuitly around current conatactor in all klystron modulator has to be improved.

(d) Some C-band klystrons have paracitic self-oscillation and multi-pacting problem. Careful study is required to identify physical origin of this problem, followed by correction to the next version of C-band klystrons.

(2) Future R&D

Machine repetition frequency of SACLA is currently limited to 60 pps as designed. Higher pulse rate is required for various experiments; such as pump-prove, or spectoroscopy. Hardware R&D to raise machine repetition frequency is one of the most important subjects, which will include

(a)High-repetition klystron tube.

(b)Higher average power klystrom modulator, where traditional thyratron tube will become unrealistic because of unstable plasma density due to limitation of H2-gas feeding at higher repetition operation. We need to develop reliable solidstate klystron modulator.

(c)Improve power efficiency on the whole system to lower the total energy consumption.

(d)Beam diagnostic system for higher repetition.

H. Curriculum Vitae (Chief Scientist)

NAME: Tsumoru Shintake

DATE OF BIRTH: Dec. 28, 1955

EDUCATION:

1974-1977: Nuclear Energy Engineering, University of Kyushu, Japan
1978-1979: Diploma thesis work: Development of EBIS ion source. University of Kyushu, Japan
1980-1983: PhD thesis work, Development of Microwave Undulator, visiting student at KEK.

ACADEMIC DEGREES: Dr. PhD Eng.

APPOINTMENTS:

1983-1992: Research Associate, Accelerator Division, TRISTAN Beam Monitor, KEK
1992-2002: Associate Professor, Accelrator Division, KEK
2002-: Chief Scientist, Advanced Electron Beam Physics Laboratory, RIKEN
2006-2010: Group leader for accelerator technical R&D and main accelerator construction team leader for X-ray FEL/SPring-8

1990-1991: Visiting physicist at Frascati Laboratory, Rome Italy
Injector design work for LISA-FEL project.
1992-1995: Joint project FFTB-SLAC collaboration, Achievement of Nano-meter Spot-size Monitor at 60 nm spot (Shintake Monitor).
1996-2002: C-band R&D group leader at KEK
(35 MV/m at 5712 MHz→ now used in SPring-8/XFEL)
2002-2005: R&D leader for SCSS project, RIKEN
2006: First lasing at 49 nm in SCSS, using CeB6 gun, C-band and In-Vacuum Undulator

ACADEMIC ACTIVITIES:

1995: US Particle Accelerator School Award “Achievement of Nanometer Spot Size Monitor at FFTB SLAC”
1996: Japanese Accelerator Award, same citation as above
2007: RIKEN award for First Lasing of SCSS FEL
2007: RIKEN award for education “Shintake School”
2008-: International Organizing Committee of “The 1st International Particle Accelerator Conference (IPAC2010)”
2009-: NLS international Technical Advisory Committee

2. Photon Science Research Division

2-1. Structural Biophysics Laboratory/宮野構造生物物理研究室

Chief Scientist; Masashi Miyano, Dr. Science / 理学博士
Since April 1, 2000

A. Research Topics (Highlights)

1. Structural and functional studies of lipid-related proteins, including integral membrane proteins, as the foundation for basic and applied medicinal sciences.

The Structural Biophysics Laboratory participated Hawaii GPCR workshop coordinated by Brian and Tong Sun Kobila at Stanford University as an organizer, and promoted for young scientists in the field to participate the meeting for exchange cutting-edge sciences and new technologies for the GPCR structural biology approaches as the medicinal important targets.

In our structural studies on GPCR, Tetsuya Hori *et al.* (2010) can now produce the enough solubilized BLT1 protein with ligand binding ability for the structural studies as drug target. The production of the lipid mediator receptor attained using a thermally stabilized mutants as well as elimination of posttranslational modifications, whereas the all rhodopsin-type GPCRs except for rhodopsin itself with built-in vitamin A derivative as reverse agonist are known unstable during solubilization from embedded membrane. Hori designed further thermally stable mutant BLT1, and it may be more appropreate for the structural studies. Hori and Sugahara are starting the crystallization trials of ligand complex routinely by various methods including the specific Fab complex co-crystallization as well as detergent effects.

In the MAPEG (Membrane Asociated Proteins in Eicosanoid and Glutathione metabolism) structural studies as important drug target, Saino and Ago *et al.* (2011) achieved high resolution human leukotriene C_4 synthase (LTC_4S) structure equipped with a Sagittal mirror under developing at BL26B1 in collaboration with Research Infrastructure Group. The structures and kinetic profiles of the several arginine residues lead the confirmation of two Arginine side chain activated catalysis to conjugate the hydrophilic GSH and Amphiphilic LTA_4 in highly site-selective and stereo-selective manner. It may contribute the more selective and specific therapeutics for allergy to pollen (Press release 2011.3.2). Further inspection of the high resolution LTC_4S structure, Miyano *et al.* (2010) proposed that the “wedged” water molecule at the transmembrane helix kink contributes functionally as well as structurally.

Microsomal prostaglandion E synthase 1 and its chimera mutants were crystallized. They were tiny and diffracted only low resolution. The improvement of crystallization is in progress.

PGE_2 and LTC_4 specific monoclonal antibodies are tools for physiological pathophysiological clinical monitoring and possible therapeutic efficacy because these major proinflamatory Eicosanoids may indicate exaggeration of disease. In the way of better and higher selectivivity and affinity their single chain Fab design in collaboration (Kakawaki et al. 2010), Thier Fab fragments complex with corresponding lipid and other structurally related ones including each apo form were determine at high resolution using newly established purification which can separate multiple heterogeneities of Fab products. PGE_2–specific Fab sample without separated heterogeneities had gave PGE_2 but not apo form or PGE_1 complex (Kurahashi & Sugahara *et al.*, 2008). This technology was applied for the membrane protein specific Fab complex preparation.

B. Research Subjects

(1) Structural and Functional Studies on Lipid mediaror related Proteins
(2) Structural elucidatioin based on High-resolution crystal structures with thermodynamic profile.
(3) GPCR structural studies.

C. Projects

Project name	Category	Started	Completed
MAPEG	Institute Program / Kakenhi(Grants-in-Aid for Science Research)/	2007	2012
GPCR BLT1	Institute Program	2007	2012
GPCR 2	Private Foundation	2008	2012
Lactamase	Institute Program	2008	2011

D. Members

as of March 1st, 2011

	number	Name
Research Scientist	5	Masashi Miyano, Hideo Ago, Tetsuya Hori, Mitsuaki Sugahara, Hiromichi Saino
Technical Scientist	0	
Research Staff	1	Yoko Ukita
Techical Staff	0	
Visiting Researchers	26	
Trainees	17	

E. Funding

(million yen)

	FY2008	FY2009	FY2010
Laboratory budget from RIKEN	19	18	16
Competitive fund in RIKEN	8	16	10
Competitive fund outside RIKEN	11	5	2
Other fund from University, Private foundations etc.	11	11	11

F. Research Output

	FY2008	FY2009	FY2010
International Publications	13	12	11
Publications in Japanese	4	1	0
Oral Presentations	4	29	21
Patent Applications	0	0	0

a. Papers

(1) Saino, H., Ukita, Y., Ago, H., Irikura, D., Nisawa, A., Ueno, G., Yamamoto, M., Kanaoka, Y., Lam, B.K., Austen, K.F., and Miyano, M. The Catalytic Architecture of Leukotriene C_4 Synthase with Two Arginine Residues. *J Biol Chem* (2011) **in press**

(2) Miyano M, Ago H, Saino H, Hori T, Ida K. Internally bridging water molecule in transmembrane α-helical kink. *Curr Opin Struct Biol* (2010) **20**:456-463.

(3) Hori T, Sato Y, Takahashi N, Takio K, Yokomizo T, Nakamura M, Shimizu T, Miyano M. Expression, purification and characterization of leukotriene B_4 receptor, BLT1 in *Pichia pastoris*. *Protein Expr Purif.* (2010) **72**:66-74.

(4) Kawakami Y, Yamashita C, Kashiwase Y, Morinaka T, Suzuki-Yamamoto T, Yamashita H, Kimoto M, Tsuji H, Kurahashi Y, Daiyasu H, Toh H, Sugahara M, Miyano M, Yamamoto S, Takahashi Y. Functional expression of single-chain antibody to leukotriene C_4. *Biochem Biophys Res Commun.* (2010) **392**:421-425.

(5) Nitanai Y, Shimamura T, Uchiyama T, Ishii Y, Takehira M, Yutani K, Matsuzawa H, Miyano M. The catalytic efficiency (k_{cat}/K_m) of the class A β-lactamase Toho-1 correlates with the thermal stability of its catalytic intermediate analog. *Biochim Biophys Acta*. (2010) **1804**:684-691.

(6) Kumasaka T, Aritake K, Ago H, Irikura D, Tsurumura T, Yamamoto M, Miyano M, Urade Y, Hayaishi O. Structural basis of the catalytic mechanism operating in open-closed conformers of lipocalin type prostaglandin D synthase. *J Biol Chem.* (2009) **284**:22344-22352.

(7) Yasuda D, Okuno T, Yokomizo T, Hori T, Hirota N, Hashidate T, Miyano M, Shimizu T, Nakamura M. Helix 8 of leukotriene B4 type-2 receptor is required for the folding to pass the quality control in the endoplasmic reticulum. *FASEB J.* (2009) **23**, 1470-1481.

(8) Kurahashi Y, Sugahara M, Ago H, Aoyama S, Takahashi N, Takio K, Katsukawa M, Yamamoto S, Miyano M. Crystallization and preliminary diffraction studies of prostaglandin E2-specific monoclonal antibody Fab fragment in the ligand complex. *Acta Crystallogr Sect* F (2008) **64,** 1027-1030.

b. Oral Presentations (* Invited presentation)

(1) Ago H. : "Crystal structure of leukotrien C_4 synthase responsible for the cystenyl leukotriene synthesis. SPring-8 GPCR Symposium, Hyogo, (2008).

(2) Miyano M. : "Strutural Studies on GPCRs : New Era of Structursl Biology on Medicinal target Membrane Proteins." 8th Ann. Meeting of Protein Society of Japan. Tokyo, June (2008).*

(3) Miyano M. : "Crystal structures of recombinant membrane proteins: SR protein crystallography for drug discovery." SAR Forum, Tokyo, June (2008).*

(4) Miyano M. : " Eicosanoids related proteins including their receptors for drug discovery." APS, Chikago, & UCLA USA, ESRF, France Sep. (2008).

(5) Ago H. : "Novel structure of leukotriene C_4 synthase." JSPS 169 Seminar, Tokyo, Oct. (2009).*

(6) Miyano M. : "Lipid Structural Biology toward the Structre-based Drug Design." Nobel Forum 2009, Bejing, China, Dec. (2009).*

(7) Ago H. : "Synchrotron Radiation Structural Biology of Proteins Functioning at Biological Membrane." 27th Naito Foundation Symposium, Jul. (2010).*

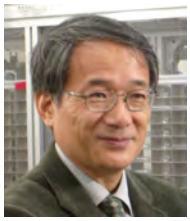
(8) Miyano M. : Visualization of Waters and Lipids in Protein Cryastals." ASI-SPring-8 Joint Symposium 2010, Wako, Japan, Sep. (2010).*

(9) Miyano, M. : "High resolution crystal structures of A-type GPCRs" GPCR workshop, Hawaii USA, Dec. (2010).*

G. Future Plan

Protein imaging contributes to not only the advancement of basic life science but also has practical applications in fields such as drug discovery. For this reason, the imaging of proteins that are involved with lipids, including membrane-embedded proteins, is a major research area at various levels ranging from sub-atomic to cellular and employing numerous methods: X-ray crystallography, neutron crystallography, NMR, electron microscopy including the diffraction method, single molecule imaging, and fluorescence imaging. The appearance and shape of a protein molecule directly links to its molecular function, just as the appearance of cells can indicate their differentiation, as shown again recently in iPS cells (Aoi & Nakayama *et al, Science* 2008). The structures of proteins stranded at interfaces of aqueous solutions and lipid membranes remain to be elucidated in detail due to the difficulties associated with sample preparation and handling. We seek to obtain methods for integrated protein imaging in such heterologous environments, and XFEL is a good candidate light source for this purpose. Thus, our prospective goal is to provide integral images of proteins within specific environments to elucidate their molecular functions relative to their biological functionalities, through the working fields of major methodologies with the futuristic XFEL light source as well as the synchrotron radiation source of SPring-8, in technological and scientific collaborations both inside and outside of RIKEN.

H. Curriculum Vitae (Chief Scientist)



NAME: Masahi Miyano

DATE OF BIRTH: December 5, 1953

EDUCATION:

1972 - 1976	Tohoku University, Faculty of Science, Biological Institute
1976 - 1978	Tohoku University Graduate School, Biological Science (MS)
1987 - 1989	Post Doc. Study Univ. California, San Diego (Professor Xuong).

ACADEMIC DEGREES: Dr. Science

APPOINTMENTS:

1978-1987	Researcher, Central Research Institute Japan Tobacco & Salt Coop. (Present name: JT)
1989-1994	JT Senior Researcher
1992-1995	Team Leader of Protein Crystallography, JT Life Science Lab.
1994-2000	JT Special Senior Researcher
1993-1995	Head of Visiting Scientist, Agroun Pharmaceutical at San Diego (Present: Pfizer San Diego)
1995-2000	Head Protein Crystallogr. for SBDD, JT Cent. Pharm. Res. Inst.
2000-	RIKEN Chief Scientist, Head of Structural Biophysics Laboratory
2000-2002	Group Head, RIKEN SR Structural Biology Group
2001-2002	Member of Res. Commit for the IPR protection from post-genomic researches, Inst. Intellect. Property
2001-	Expert member of Congress on Kansai Bio Promotion
2001-	Committee member, Bio Promotion committee, The Osaka Chamber of Commerce & Industry
2001-2003	Director, RIKEN Highthroughput Factory
2001-2003	Group director, RIKEN Structural Genomics/Proteomics Initiative
2001-2002	Guest lecturer Graduate School of Pharmacology, Kyoto University,
2003-prsent	Guest lecturer of School of Medicine, University of Tokyo
2005	Guest lecturer of Internat. Grad, Sch. of Arts Sci., Yokohama City Univ.
2006	Guest lecturer of Grad. Sch. of Agribio-science, Nagoya University
2007-2008	Guest lecturer of Graduate School of Medicine, Kyushu University

ACADEMIC ACTIVITIES:

Japan Biophysics Society
Japan Crystallographic Society
Japan Biochemical Society
Japan Molecular Biological Society
Japanese Society for Synchrotron Radiation Research
American Crystallographic Association
American Society for Biochemistry and Molecular Biolo

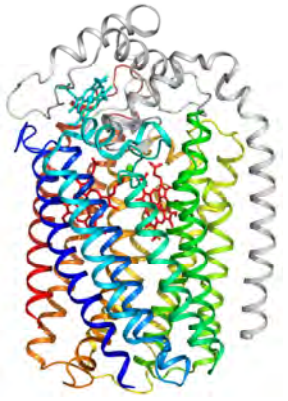
2-2. Biometal Science Laboratory / 城生体金属科学研究室

Chief Scientist; Yoshitsugu SHIRO, Dr. Eng. / 城　宜嗣
Since April 2000

A. Research Topics (Highlights)

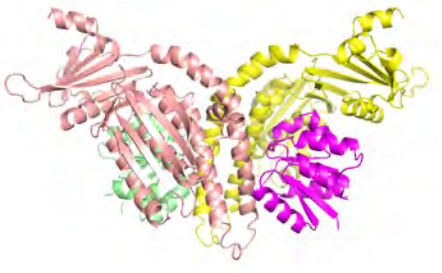
1. Bacterial Nitric Oxide Reductases

We succeeded in crystallization and structural determination of membrane-integrated bacterial nitric oxide redutases NOR by using SPring-8 BL. NOR is an iron-containing enzyme involved in denitrification, which is a kind of anaerobic respiration of microorganism. Since NOR is closely related to the molecular evolution of respiratory enzymes, it has been believed to share the common ancestor with cytochrome oxidases in aerobic respiration (O_2 + $4H^+$ + $4e^-$ → $2H_2O$). In addition, environmental science also pays much attention to NOR, because the reactant NO of the enzymatic reaction is one of the air pollutant NOx having a high cyto-toxicity, and the product N_2O is not only a greenhouse gas, more powerful by 310 times than carbon dioxide CO_2, but also a main contributor for depletion of the ozone layers. On the basis of their molecular structures, we discussed the molecular mechanism of their catalytic reaction ($2NO + 2H^+ + 2e^-$ → $N_2O + H_2O$); i.e., the N-O bond cleavage and the N-N bond formation in association with electron/proton transfer. By comparing the NOR structure with those of aerobic and micro-aerobic respiratory enzymes in detail, we can start to discuss their molecular evolution; i.e., upon emergence of O_2 on the earth, how the enzymatic function was converted from the NO reduction to the O_2 reduction, and how the enzyme acquired the proton pumping ability.



2. Complex of Histidine Kinase and Response Regulator in Two-component System

We determined the crystal structure of the complex of thermophilic bacterial histidine kinase (HK) and its cognate response regulator (RR) of the two-component regulatory system by combinational use of X-ray crystallography and small angle scattering techniques. This sensory system is ubiquitous in bacteria, fungi and plants to adapt their environmental changes through the protein phosphorylation by ATP, phospho-transfer reactions and then gene expression/protein activation. For example, the O_2-sensor protein FixL in root nodule regulates the expression of the N_2 fixation enzyme, nitrogenase, in response to the surrounding O_2 tension. On the basis of the structure we determined, we proposed inter-domain and inter-molecular signal transduction in this system from HK (sensor domain → catalytic domain → dimerization domain) to RR.



3. Iron-Enzyme Involved in Tryptophan Metabolism

In 2006, we reported crystal structure of indoleamine 2,3-dioxygenase (IDO), which is involved in tryptophan (Trp) metabolism in mammal. IDO catalyzes insertion of two atomic oxygen of O_2 into the substrate Trp by virtue of the iron at the active site. On the basis of the molecular structure we reported, the molecular mechanism of this physiologically significant

chemical reaction was studied by vibrational spectroscopic techniques and method of quantum-chemical theory.

4. Structural Characterization of Fluorescent Properties of GFP-like Proteins

GFP (green fluorescent protein)-like proteins exhibit a variety of fluorescence (color, intensity, Stork-shift, photochromism, and so no). To understand how such fluorescent properties can be regulated in atomic level, we determined crystals structures of 25 fluorescent and 4 non-fluorescent proteins and revealed interaction of the chromophores with their surrounding protein part. This is the joint project with Miyawaki's group in Brain Science Institute of RIKEN.

B. Research Subjects

(1) Structural and Functional Analyses of Metal-containing Enzymes Involved in Biological Reactions
(2) Structural and Functional Analyses of Metal-containing Proteins Involved in Cellular Signal Transduction
(3) Structural and Functional Analyses of Proteins Involved in Dynamics of Metals in Biology
(4) Development and Application of New Technologies for Protein Structural Determination

C. Projects

Project name	Category	Started	Completed
Molecular Science of Metals in Biology	Institute Program	2006	2012
Vibrational Spectroscopic Study on Short-lived Respiratory Enzyme-Substrate Complex	MEXT, Grant-in-Aid for Scientific Research on Priority Areas	2006	2009
Structure and Reaction Mechanism of Dioxygen Activation in Human Dioxygenase	MEXT, Grant-in-Aid for Young Scientists (B)	2007	2008
Molecular Evolution of Respiratory Enzymes	MEXT, Grants-in-Aid for Science Research (B)	2007	2009
Crystallography of Enzymes Involved in Bio-synthesis of Indole-compounds	Private Foundation	2008	2008
Molecular Science and Inhibitor Search of Tryptophan Metabolism in Mammals	Private Foundation	2008	2008
Structural Dynamics of Deoxygenates Evaluated by Time-resolved Resonance Raman Spectroscopy	MEXT, Grant-in-Aid for Scientific Research on Priority Areas	2008	2009

Functional Conversion and Molecular Evolution of Respiratory Enzymes from NO Reduction to O_2 Reduction	MEXT, Grants-in-Aid for Science Research (A)	2009	2012
Regulation of High Specificity and Function of Biological Reaction Sphere	MEXT, Grants-in-Aid for Science Research on Innovative Areas	2010	2014
Molecular Mechanism of the Catalytic Reaction by Bacterial Nitric Oxide Reductase: Comparison with Oxygen Reduction	MEXT, Grant-in-Aid for Young Scientists (B)	2010	2011

D. Members

as of March 1st, 2011

	number	Name
Research Scientist	9	Yoshitsugu Shiro, Hiro Nakamura, Hiroshi Sugimoto, Akihiro Kikuchi, Thirumananseri Kumarevel, Tsutomu Mikawa, Tamao Hisano, Takehiko Tosha, Yoko Ito
Technical Scientist	0	
Research Staff	0	
Technical Staff	0	
Visiting Researchers	35	
Trainees	19	

E. Funding

(million yen)

	FY2008	FY2009	FY2010
Laboratory budget from RIKEN	23	23	24
Competitive fund in RIKEN	14	10	5
Competitive fund outside RIKEN	18	24	43
Other fund from University, Private foundations etc.	5	1	1

F. Research Output

	FY2008	FY2009	FY2010
International Publications	5	11	6
Publications in Japanese	1	2	1
Oral Presentations	9	6	6
Patent Applications	0	0	0

a. Papers

(1) L. W. Chung, X. Li, H. Sugimoto, Y. Shiro, K. Morokuma: "Density Functional Theory Study on a Missing Piece in Understanding of Heme Chemistry: The Reaction Mechanism fro Indoleamine 2,3-dioxygenase and Tryptophan 2,3-dioxygenase" *J. Am. Chem. Soc.* **130**, 12299-12309 (2008)
(2) A. Kikuchi, E. Fukumura, S. Karasawa, H. Mizuno, A. Miyawaki, Y. Shiro: "Structural Characterization of a Thiazoline-containing Chromophore in an Orange Fluorescent Protein, Monomeric Kusabira Orange" *Biochemistry*, **47**, 11573-11580 (2008)
(3) E. Fukumura, H. Sugimoto, Y. Misumi, T. Ogura, Y. Shiro: "Cooperative Binding of L-Trp to Human Tryptophan 2,3-Dioxygenase: Resonance Raman Spectroscopic Analysis" *J. Biochem.* **145**, 505-515 (2009)
(4) A. Kikuchi, E. Fukumura, S. Karasawa, Y. Shiro, A. Miyawaki: "Crystal Structure of a New Cyan Fluorescent Protein and Its Hue-shifted Variants" *Biochemistry* **48**, 5276-5283 (2009)
(5) Y. Wang, H. Chen, M. Makino, Y. Shiro, S. Nagano, S. Asamizu, H. Onaka, S. Sason: "Theoretical and Experimental Studies of the Conversion of Chromopyrrolic Acid to an Antitumor Derivative by Cytochrome P450 StaP: The Biological Role of Water Molecules" *J. Am. Chem. Soc.* **131**, 6748-6762 (2009)
(6) S. Yamada, H. Sugimoto, M. Kobayashi, A. Ohno, H. Nakamura, Y. Shiro: "Structure of PAS-linked Histidine Kinase and the Response Regulator Complex" *Structure* **17**, 1333-1344 (2009)
(7) T. Sakaki, H. Sugimoto, K. Hayashi, K. Yasuda, E. Munetsna, M. Kamakura, S. Ikushiro, Y. Shiro: "Bioconversion of Vitamin D to Its Active Form by Bacterial or Mammalian Cytochromes P450" *Biochim. Biophys. Acta* **1814**, 249-256 (2010)
(8) L. W. Chung, X. Li, H. Sugimoto, Y. Shiro, K. Morokuma: "ONIOM Study on a Missing Piece in Our Understanding of Heme Chemistry: Bacterial Tryptophan 2,3-Dioxygenase with Dual Oxidants" *J. Am. Chem. Soc.* **132**, 11993-12005 (2010)
(9) S. Yanagisawa, H. Sugimoto, Y. Shiro, T. Ogura: "A Specific Interaction of L-Tryptophan with CO of CO-Bound Indoleamine 2,3-Dioxygenase Identified by Resonance Raman Spectroscopy" *Biochemistry* **49**, 10081-10088 (2010)
(10) T. Hino, Y. Matsumoto, S. Nagano, H. Sugimoto, Y. Fukumori, T. Murata, S. Iwata, Y. Shiro: "Structural Basis of Biological N_2O Generation by Bacterial Nitric Oxide Reductase" *Science* **330**, 1666-1670 (2010)
(11) H. Sugimoto, O. Takikawa, Y. Shiro: "Tryptophan Catabolism by Heme Dioxygenases" in *Handbook of Porphyrin Science* (K. M. Kadish, K. M. Smith, R. Guilard, Eds.) Vol. 5, Chapter 24, pp.71-122 (2010)
(12) Y. Shiro, S. Nagano: "NO Chemistry by Heme-Enzyme" in *Handbook of Porphyrin Science* (K. M. Kadish, K. M. Smith, R. Guilard, Eds.) Vol. 5, Chapter 25, pp.123-163 (2010)

b. Oral Presentations (* Invited presentation)

(1) Shiro, Y., Nagano, S., Matsumoto, Y.: "Fungal and Bacterial Nitric Oxide Reductases: Their Structures and Reaction Mechanisms" *Fifth International Conference on Porphyrins and Phthalocyanines*, Moscow, Russia, July (2008) *
(2) Matsumoto, Y., Nagano, S., Shiro, Y.: "Fungal and Bacterial Nitric Oxide Reductases: Their Structures and Reaction Mechanisms" *4th Asian Biological Inorganic Chemistry Conference*, Jeju, Korea, Nov. (2008) *
(3) Shiro, Y.: "Structure and Function of Nitric Oxide Reductases; Chemistry of NO

Reduction and N_2O formation" *1st Korea-Japan Seminars on Biomolecular Sciences - Experiments and Simulations*, Seoul, Korea, Feb.-Mar. (2009) *

(4) Shiro, Y.: "Structure and Function of Nitric Oxide Reductases; Chemistry of NO Reduction and N_2O Formation" *14th International Conference of Biological Inorganic Chemistry*, Nagoya, Japan, July (2009) *

(5) Shiro, Y., Hino, T., Matsumoto, Y., Nagano, S., Sugimoto, H., Tousha, T.: "Nitric Oxide Reductases: Chemistry of N-O bond Cleavage and N-N Bond Formation" *Sixth International Conference on Porphyrins and Phtalocyanines*, New Mexico, USA, July (2010) *

(6) Shiro, Y., Nakamura, H., Ito, Y., Sugimoto, H.: "Two-Component Regulatory System: Cellular Signal Transduction Systems Sensing Exogenous Stimuli" *2010 International Chemical Congress of Pacific Basin Societies*, Honolulu, USA, Dec. (2010) *

(7) Hino, T., Matsumoto, Y., Pisliakov, A., Nagano, S., Sugimoto, H., Sugita, Y., Shiro, Y.: "Molecular Structures and Mechanism of Bacterial Nitric Oxide Reductase" *Third Korea-Japan Seminars on Biomolecular Sciences - Experiments and Simulations*, Jeju, Korea, Feb. 28 (2011) *

G. Future Plan

Transition metals in biology, as known as "biometal", play physiologically crucial roles in biological processes. Metal-binding proteins and enzymes contribute to conversion of bio-materials, bio-information and bio-energy with very high efficiency and high specificity under mild condition of temperature, pressure and pH. We specially focus on the metal-binding proteins and enzymes which are involved in activation/binding of small gas molecules such as O_2, NO, ethylene (plant hormone) and so on. Through study on the structure-function relationship of these proteins, we would like to learn much about the chemistry of biological processes/reactions in atomic level, leading to establishment of a new interdisciplinary scientific field such as "Biofunction Mimetic Chemistry", by which we will accomplish to develop novel materials and catalysts.

We also have much interest in structure/functions of proteins related to dynamics of biometals. We are now challenging to elucidate the structures and functions of metal-transporters and metal-sensors in biology by combinational uses of X-ray techniques at SPring-8 including crystallography, small angle scattering and absorption/fluorescent spectroscopy at SPring-8. The former proteins transport metal ions or metal-complexes across the cellular membrane to control their concentration inside the cells which can be monitored by the later proteins. Since some metal elements are indispensable for our life, these transporting and sensing systems are essential to strictly control their concentration in our body; both excess and shortage would cause to damage the cells. In addition to the biological, physiological and pharmaceutical significance, this project is challenging, from structure-biological points of view, because many of our targets are membrane-bound proteins, multi-domain proteins, and the protein-complexes. In the course of investigation of these targets, we will try to develop new technologies and methodologies, which will contribute to progress of the bio-molecular science.

H. Curriculum Vitae (Chief Scientist)

NAME: Yoshitsugu SHIRO

DATE OF BIRTH: November 6, 1956

EDUCATION:

1976 - 1980: Faculty of Engineering, Kyoto University
1980 - 0985: Graduate School of Engineering, Kyoto University

ACADEMIC DEGREES: Dr. Eng.

APPOINTMENTS:

1985 - 1987: Postdoctoral Fellowship of JSPS
1987 - 1993: Research Scientist, RIKEN
1993 - 2000: Senior Research Scientist, RIKEN
2000 - date : Chief Scientist, RIKEN Harima Institute/ RIKEN SPring-8 Center
1991 - 1992: Visiting Scholar, Department of Chemistry, Stanford University, USA
1999 – date : Visiting Professor, Graduate School of Science, Himeji Institute of Technology (University of Hyogo), Japan
2000 : Visiting Professor, Institute of Multidisciplinary Research on Advanced Materials, Tohoku University, Japan
2005 - 2007: Visiting Professor, Graduate School of Science, Kyoto University, Japan
2006 - date: Visiting Professor, Graduate School of Science, Osaka University, Japan
2007 : Visiting Professor, Graduate School of Science, Nagoya University, Japan

ACADEMIC ACTIVITIES:

Chemical Society of Japan
The Japanese Biochemical Society
The Biophysical Society of Japan
Protein Science Society of Japan
2000: Local Program Committee of "The 11th International Conference on X-ray Absorption Fine Structure (XAFS IX)"
2004: Local Steering Committee of "The 8th International Conference on Biology and Synchrotron Radiation (BSR2004)"
2009: Chair of Program Committee of "14th International Conference on Biological Inorganic Chemistry (ICBIC14)"
2009: Organizing Committee of "16th International Conference on Cytochrome P450"
2009 - date: Board member of Protein Science Society of Japan

2-3. Structural Materials Science Laboratory / 高田構造科学研究室

Chief Scientist Masaki TAKATA, Ph.D. / 高田 昌樹
Since April 2006

A. Research Topics (Highlight)

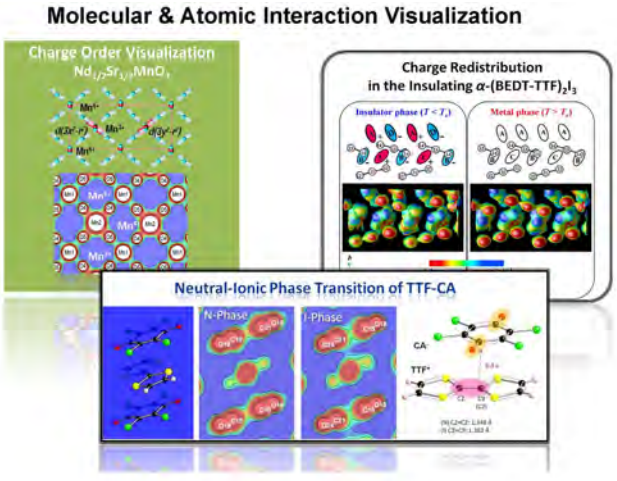
The research goal of the laboratory is to develop innovations in Structural Materials Science using Synchrotron Radiation (SR) X-ray diffraction to allow visualization of interactions between atoms and molecules in advanced materials exhibiting novel functional properties. The achievement of this goal will evolve the Structural Materials Science from precise structure determination into a direct investigation of structure-property correlations in terms of electrostatic potential (EP). The scientific targets include extensive topical research areas such as superconductivity, metal-insulator/neutral-ionic transition, photo-induced phenomena, thermoelectric materials, and phase change materials. To accomplish this goal, methodologies for both X-ray diffraction experiment and data analysis techniques have been developed. We have constructed a precise SR powder diffractometer at BL44B2, a single crystal diffractometer at BL02B1, and an X-ray pinpoint structure measurement system at BL40XU. A method for EP imaging method using diffraction data has also been developed using our Maximum Entropy Method (MEM) analysis program, ENIGMA. Following are recent examples of topics explored:

1. Visualization of the charge transfers through the M-I transition

To investigate a sample's structural basis at an electron density level of a metal-insulator (M-I) transition of α-(BEDT-TTF)$_2$I$_3$ at 135 K, the charge density mapping and EP imaging were performed using Synchrotron Radiation X-ray powder diffraction. The precise charge density that was obtained clearly revealed a significant charge transfer between the I_3 and ET molecules through the M-I transition. In the EP, we found the localized change around the I_3 molecule representing the existence of a charge order of the neighboring ET molecule at a low temperature. The EP on the cross-section of the I_3 molecule successfully allowed visualization of the characteristic conducting layer configuration of ET molecular arrays detached by the insulator I_3 layers. In addition, directional electric field analysis allowed visualization of a potential shield breaking between I_3 insulating and ET conducting channels associated with the local change of electrostatic interaction. Our present findings in terms of the electrostatic interaction between I_3 and ET molecules will lead to a fuller understanding of the M-I transition of α-(BEDT-TTF)$_2$I$_3$.

2. Visualization of localized electrostatic interaction in the TTF-CA ionic phase

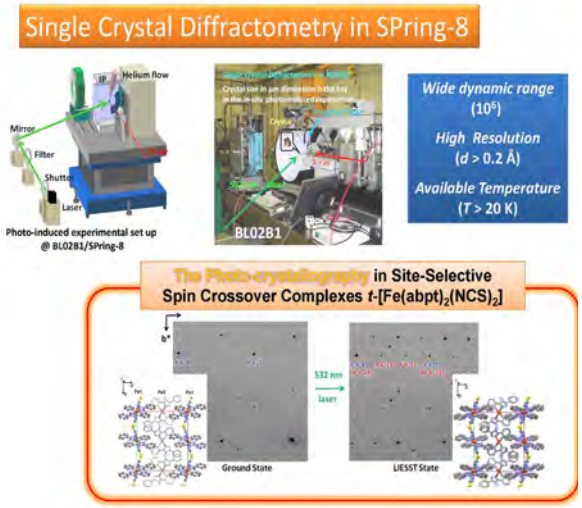
One of the typical Neutral-Ionic Transition (NIT) materials, tetrathiafulvalene-p-chloranil (TTF-CA), was investigated with EP imaging using the MEM program, based on data from synchrotron radiation powder diffraction data. The EP obtained revealed the structural features of charge transfer from the TTF molecule to the CA molecule



through the thermally induced NIT (Tc = 81 K). From the charge density change, the degree of charge transfer (CT) was evaluated as 0.30(2) e through the NIT. In the EP, it was found that a significant potential valley appeared at the inter-molecular region connecting between the C2=C9 bonding part in TTF and the C15(21)-O18(24) part in CA. The present findings indicate the existence of a distinct local molecular interaction between TTF and CA in the I phase.

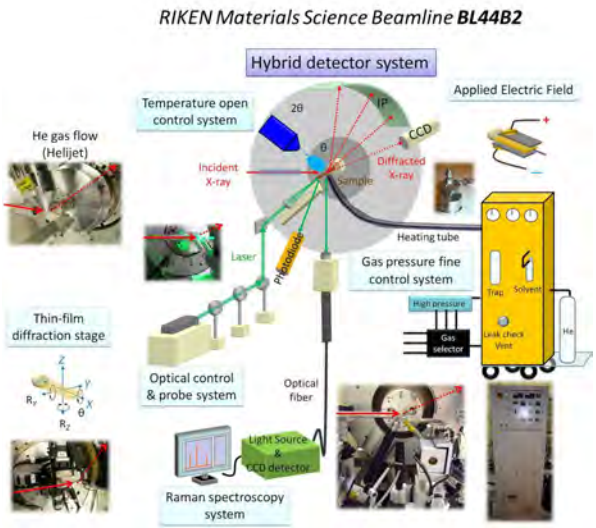
3. The photo-induced commensurate modulated structure in a site-selective spin crossover complex *trans*-[Fe(abpt)$_2$(NCS)$_2$]

The photo-induced superstructure of polymorph C of *trans*-[Fe(abpt)$_2$(NCS)$_2$] (abpt = 4-amino-3,5-bis(pyridin-2-yl)-1,2,4-triazole) is discovered as a commensurate modulated structure by single-crystal X-ray diffraction under irradiation. The crystal structure at 25 K before the photo-irradiation is composed of two crystallographically independent iron molecules, one of which exhibits a high spin (HS) state and the other at low spin (LS) state. Under green laser light (λ = 532 nm) irradiation, the LS molecule (Fe1) is found to be excited to a metastable HS state, giving rise to a commensurate tripled superstructure along the c axis. In addition, it is confirmed that this modulation persists up to the HS→LS relaxation temperature beyond 52K. Our structural findings suggest a high correlation between that the structural modulation and the site-selective LS→HS excitation.



4. Development of a high-resolution Debye-Scherrer camera for Visualization of electrostatic interactions in materials

In order to visualize molecular interactions using experimental electrostatic potential analysis, we optimized the optical parameters and developed a high-resolution Debye-Scherrer camera at the RIKEN materials science beamline (BL44B2 at SPring-8). For this purpose the camera was equipped with a hybrid X-ray detector system. One is the conventional detector, with the imaging plate readout off-line to carry out high d (interplanar spacing)-resolution measurements. The other is a CCD detector, which can be operated in a camera at variable distances for high angle-resolution measurements. In addition we have been developing an in-situ system for properties measurement to visualize electrostatic interactions completely synchronized with material functions.



B. Research Subjects

(1) Electrostatic potential imaging of advanced materials by SR diffraction
(2) Precise electron density mapping of proteins by MEM
(3) Structural materials science of nano-bio materials by SR small angle scattering
(4) Visualization of nano-level material reactions by time resolved X-ray diffraction
(5) Electron spin density mapping of magnetic materials by SR scattering

C. Projects

Project name	Category	Started	Completed
Charge density studies of molecule-adsorbed nanomaterials	MEXT, Grant-in-Aid for Scientific Research on Priority Areas	2004	2007
X-ray pinpoint structural measurement ―Development of spatial- and time-resolved structural studies for nanomaterials and devices―	JST, CREST	2004	2009
Development of a femtoseconds microscope and an electrostatic potential imaging method	MEXT, XFEL Research Promotion Program	2006	2010
Development of Carbon-Neutral Energy Cycles by Highly Selective Catalysis	JST, CREST	2010	2015
Application and design of a coordination polymer with the microporous scaled down to the single H_2 molecule size for highly controled storage	Private Foundation	2010	2011

D. Members

as of April 1, 2011

	number	Name
Research Scientists	4	Masaki Takata, Kenichi Kato, Hiroyuki Ohsumi, Takashi Kosone
Technical Scientists	0	
Research Staff	0	
Technical Staff	0	
Visiting Researchers	47	
Trainees	33	

E. Funding

(million yen)

	2006	2007	2008	2009	2010
Government Budget	52	68	29	39	26
Grants	12	19	12	6	10
Private & Other Sources	0	0	0	0	0

F. Research Output

	2006	2007	2008	2009	2010
International Publications	34	30	22	24	28
Publications in Japanese	5	4	4	5	3
Oral Presentations	39	51	36	16	14
Patent Applications	0	0	0	0	0

a. Papers

(1) Takata,M.: "The MEM/Rietveld Method with Nano-Applications –Accurate Charge-Density Studies of Nano-Structured Materials by Synchrotron-Radiation Powder Diffraction", *Acta Cryst. A* **64**, 232-245 (2008).

(2) Kato, K., Morimoto, Y., Takata, M., Tanaka, H., and Hamada, N.: "Visualization of Charge Ordering in a Half-Doped Manganite by an Electrostatic Potential Analysis", *Phys. Rev. B* **77**, 081101 (2008).

(3) Zheng, X. G., Kubozono, H., Yamada, H., Kato, K., Ishiwata, Y., and Xu, C. N.: "Giant Negative Thermal Expansion in Magnetic Nanocrystals", *Nature Nanotechnology* **3**, 724-726 (2008).

(4) Makiura, R., Yonemura, T., Yamada, T., Yamauchi, M., Ikeda, R., Kitagawa, H., Kato, K., and Takata, M.: "Size-Controlled Stabilization of the Superionic Phase to Room Temperature in Polymer-Coated AgI Nanoparticles", *Nature Materials* **8**, 476-480 (2009).

(5) Kuriyama, H., Matsumoto, J., Niitaka, S., Uchida, M., Hashizume, D., Nakao, A., Sugimoto, K., Ohsumi, H., Takata, M., and Takagi, H. : " Epitaxially stabilized iridium spinel oxide without cations in the tetrahedral site", *Applied Physics Letters* **96**, 182103 (2010)

(6) Fukuyama, Y., Yasuda, N., Kamioka, H., Kim, J., Shibata, T., Osawa, H., Nakagawa, T., Murayama, H., Kato, K., Tanaka, Y., Kimura, S., Ohshima, T., Tanaka, H., Takata M. & Moritomo,Y. : "Simultaneous Measurements of Picosecond Lattice and Charge Dynamics in Co–Fe Cyanides", *Applied Physics Express* **3**, 016601 (2010)

(7) Miyazaki, J., Matsudaira, K., Shimizu, Y., Itoh, M., Nagamine, Y., Mori, S., Kim, J. E., Kato, K., Takata, M., and Katsufuji, T.: "Formation of a Three-Dimensional Network of V Trimers in $A_2V_{13}O_{22}$ (A = Ba, Sr)", *Phys. Rev. Lett.* **104**, 207201 (2010).

(8) Hosono, N., Kajitani, T., Fukushima, T., Ito, K., Sasaki, S., Takata, M., Aida, T: "Large-Area Three-Dimensional Molecular Ordering of a Polymer Brush by One-Step Processing", *Science* **330**, 808-811 (2010).

(9) Ganin, A. Y., Takabayashi, Y., Jeglic, P., Arčon, D., Potočnik, A., Baker, P. J., Ohishi, Y., McDonald, M. T., Tzirakis, M. D., McLennan, A., Darling, G. R., Takata, M., Rosseinsky, M. J., and Prassides, K.: "Polymorphism Control of Superconductivity and Magnetism in Cs_3C_{60} close to the Mott Transition", *Nature* **466**, 221–225 (2010).

(10) Kim, J., Tanaka, H., Kato, K., Takata, M., and Moritomo, Y., "Extended *d*-Electron State of $Fe(CN)_6$ Unit in Prussian Blue Analogue", *Appl. Phys. Express* **4**, 025801 (2011).

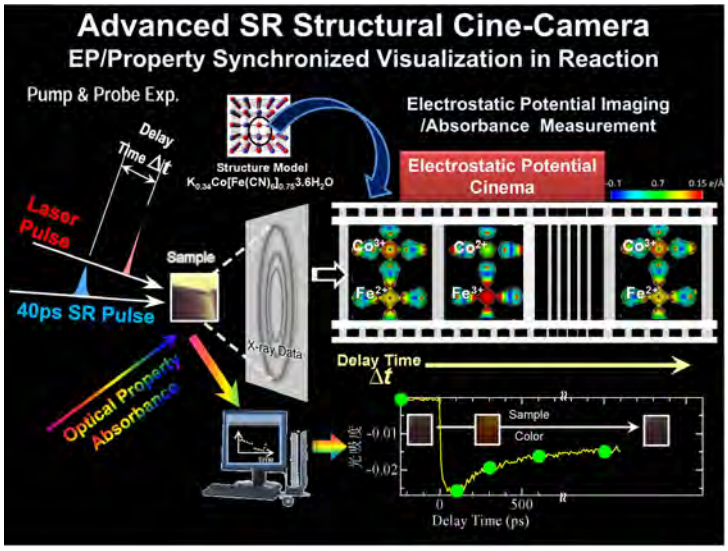
(11) Matsunaga, T., Akola, J., Kohara, S., Honma, T., Kobayashi K., Ikenaga, E., Jones, R. O., Yamada, N., Takata, M., and Kojima, R.: "From Local Structure to Nanosecond Recrystallization Dynamics in AgInSbTe Phase-Change Materials", *Nature Materials* **10**, 129-134 (2011).

b. Oral Presentations

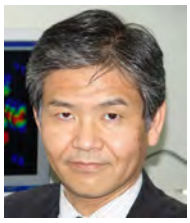
(1) Takata, M.: "Structural Basis for Fast Phase Change Mechanism of DVD Data Storage Material"(Invited Lecture), *International Conference on Materials for Advanced Technologies 2007 (ICMAT2007)*, Suntec Singapore International Convention & Exhibition Centre, Singapore, Jul. 2007.
(2) Takata, M.: "Electrostatic Potential and Electric Field Imaging by MEM Powder Diffraction Dada Analysis"(Invited Lecture), *XXI Congress and General Assembly of the International Union of Crystallography (IUCr2008)*, Grand Cube Osaka, Japan, 23-31 Aug. 2008.
(3) Kato, K.: "Bonding Electrons Visualization in Photo-Excited State using Synchrotron X-ray Powder Diffractometry"(Invited Lecture), *XXI Congress and General Assembly of the International Union of Crystallography (IUCr2008)*, Grand Cube Osaka, Japan, 23-31 Aug. 2008.
(4) Takata, M.:"Recent Progress in MEM Charge Density Study for Materials Science"(Invited Lecture), *Sagamore XVI*, Santa Fe, USA, 2-7 Aug. 2009.
(5) Takata, M.: "Current and Future Challenges in Materials Science by Synchrotron X-ray Diffraction" (Invited Lecture), *The 10th International Conference on Synchrotron Radiation Instrumentation (SRI2009)* Melbourne, Australia, 27 September - 2 Oct. 2009
(6) Kato, K.: "Molecular Interaction in Photo-Induced Phase Transition Materials Visualized by Electrostatic Potential Analysis" (Invited Lecture), *3rd International Workshop on Phase Transition and Dynamical Properties of Spin Transition Materials (PDSTM2010)*, University of Tsukuba, Japan, 6-8 Feb. 2010.
(7) Takata, M.: "Development of Synchrotron Radiation Pinpoint Structure Measurement Application to The Time Resolved Characterization of DVD"(Invited Lecture), *8th INANO Annual Meeting* , Aarhus, Denmark, 20 Jan. 2010

G. Future Plan

Our next goal is to create Live-Interaction Structural Materials Science, which will provide us live-action EP visualization of a chemical reaction monitored by the functional properties of the materials. To achieve this goal, we are planning the development of time-resolved, high resolution SR single crystal/powder diffractometry using a 100nm beam by upgrading X-ray pinpoint structural measurements. In addition to MEM and EP Imaging, the upgraded Reverse Monte Carlo (RMC) method combined with a DFT calculation will be established as an alternative data analysis technique. A preliminary application of this technique was used successfully for amorphous structure determination of the DVD materials. Our future plans should join together in the XFEL ultra-fast science using SACLA.



H. Curriculum Vitae (Chief Scientist)



NAME: Masaki TAKATA

DATE OF BIRTH: May 3, 1959

EDUCATION:

1982: Graduated from the Department of Materials Science, Hiroshima University
1984: Master's Degree from the Department of Materials Science, Hiroshima University
1988: PhD in Science from Department of Materials Science, Hiroshima University

DEGREES: Dr. Sci.

APPOINTMENTS:

1987-1997: Assistant Professor, Nagoya University
1992: Guest Scientist, Aarhus University Aarhus, Denmark
1993-1997: Lecturer, Fujita Health University
1997-1999: Associate Professor, Shimane University
1999-2003: Associate Professor, Nagoya University
2003-Present: Chief Scientist, Japan Synchrotron Radiation Research Institute
2006-Present: Chief Scientist, RIKEN Harima Institute
2007-Present: Professor, the University of Tokyo

ACADEMIC ACTIVITIES:

1999-2005: Councilor of the Crystallographic Society of Japan
2000-2002: Public-relations Manager of the Crystallographic Society of Japan
2000-2002: Editorial Committee of the Japanese Society for Synchrotron Radiation Research
2003-2004: Events Manager of the Japanese Society for Synchrotron Radiation Research
2003-2004: Councilor of the Japanese Society for Synchrotron Radiation Research
2004-2006: General Affairs Manager of the Crystallographic Society of Japan
2004-2006: Editorial Manager of the Crystallographic Society of Japan
2004-2009: Organizing Committee of IUCr2008
2005-2006: General Affairs Manager of the Japanese Society for Synchrotron Radiation Research
2006-2008: Councilor of the Crystallographic Society of Japan
2007-2008: Councilor of the Japanese Society for Synchrotron Radiation Research

II: 2-4. Materials Dynamics Laboratory / バロン物質ダイナミクス研究室

Associate Chief Scientist: Alfred Q.R. BARON, Ph.D. / アルフレド　バロン
Since: April 2006

A. Research Topics (Highlights)

1. RIKEN Quantum NanoDynamics Beamline (BL43LXU)

The RIKEN Quantum NanoDynamics (RQD) Beamline, BL4LXU, has been the primary focus of the Materials Dynamics Laboratory (MDL) since the beamline was funded in FY2009. The beamline is optimized for investigating atomic and electronic dynamics with high, <1 to ~100 meV, resolution using non-resonant inelastic x-ray scattering (IXS). It will provide unprecedented flux using a long, 15m, small-gap insertion device, with instrumentation that is designed to maximize the intensity in count-rate-limited inelastic x-ray scattering experiments. The main work of the lab has been over-seeing the design of the beamline, and the detailed fabrication of the experimental station equipment, including the spectrometers. The beamline will include two spectrometers, one for ~0.7 meV to 40 meV resolution and <1 nm^{-1} momentum resolution using a 10m 2Θ arm, and one for ~10 to 100 meV resolution and <4 nm^{-1} momentum resolution using a 2m arm. Other notable instrumentation points include an expected beam spot on the sample of about 25 microns diameter (with essentially no losses from focusing), a large, 42 element, analyzer array, and a new "temperature gradient" analyzer design to improve resolution while retaining large space for sample environments. More details can be found in section 4-4-2 and at http://user.spring8.or.jp/sp8info/?p=3138.

2. Other

The high-pressure DAC work, in collaboration with H. Fukui of Hyogo University (a former MDL post-doc) and E. Ohtani of Tohoku University has yielded good phonon spectra at pressures up to nearly 150 GPa, and papers are now being prepared. Another recent success was the measurement of very high-quality phonon spectra from a cuprate superconductor showing surprisingly large changes with temperature. Similar experiments have always suffered from extremely low rates, and while counting times (>1 day/spectrum) remain prohibitive for systematic studies, the new spectra with 1.5 meV resolution, favorably indicate one direction for new and exciting science at BL43LXU. Many of the other projects in the MDL have been slowed, or been re-focused on the new beamline. A 40 meV backscattering monochromator was constructed and tested at BL35 (with resolution in good accordance with theory) however it was decided that commissioning would be completed at BL43. Grazing incidence liquid surface scattering experiments have largely been suspended as the main person doing this (D. Ishikawa) has focused nearly entirely on BL43.

B. Research Subjects

1. Techniques & Instrumentation for High-Resolution IXS.
2. Phonons in Superconductors.
3. High Resolution Inelastic Scattering from Electronic Excitations.
4. Phonons in Multiferroic Materials
5. IXS from samples in diamond anvil cells.
6. IXS for probing dynamics of surfaces.

C. Projects

Project name	Category	Started	Completed
Single Crystal Investigations of Iron Based Superconductors	JST, TRIP	2008	2010

Investigating Superconductors with X-Rays	NEDO Grant	2008	2010

D. Members

as of March 1st, 2011

Position	Number	Names
Research Scientist	1	Alfred Q.R. Baron
Technical Scientist	0	
Research Staff	1	David S. Ellis
Technical Staff	0	
Visiting Researchers	6	
Trainees	0	

E. Funding

(million yen)

	FY2008	FY2009	FY2010
Laboratory budget from RIKEN	25	23	56
Competitive fund in RIKEN	1	3	0
Competitive fund outside RIKEN	6	1	1
Other fund from University, Private foundations etc.	2	2	1

F. Research Output

	FY2008	FY2009	FY2010
International Publications	11	6	8
Publications in Japanese	0	3	0
Oral Presentations	9	9	9
Patent Applications	0	0	0

a. Papers

(1) R. Kajimoto, H. Sagayama, K. Sasai, T. Fukuda, S. Tsutsui, T. Arima, K. Hirota, Y. Mitsui, H. Yoshizawa, A.Q.R. Baron, Y. Yamasaki, and Y. Tokura "Unconventional Ferroelectric Transition in the Multiferroic Compound $TbMnO_3$ Revealed by the Absence of an Anomaly in c-Polarized Phonon Dispersion"Physical Review Letters, 102 (2009) 247602

(2) S. Hosokawa, M. Inui, Y. Kajihara, K. Matsuda, T. Ichitsubo, W.-C. Pilgrim, H. Sinn, L. E. Gonza´lez, D. J. Gonza´lez, S. Tsutsui, and A. Q. R. Baron**,** "Transverse Acoustic Excitations in Liquid Ga" Physical Review Letters **102** (2009) 105502

(3) A.Q.R. Baron**, "**Phonons in Crystals using Inelastic X-Ray Scattering", Journal of The Spectroscopical Society of Japan, Vol. **58**, #5 (2009), **["**X線非弾性散乱による結晶中フォノンの研究", 分光研究第 5**8** 巻第 5 号(2009) pp.205-214 In Japanese, arXiv 0910.5764 (English)]

(4) D. Ishikawa and A.Q.R. Baron**,** "Temperature gradient analyzers for compact high-resolution X-ray spectrometers." Journal of Synchrotron Radiation, **17** (2010) 12-24 (also cover).

(5) C.-H. Lee, K. Kihou, K. Horigane, S. Tsutsui, T. Fukuda, H. Eisaki, A. Iyo, H. Yamaguchi, A.Q.R. Baron, M. Braden and K. Yamada "Effect of K Doping on Phonons in $Ba_{1-x}K_xFe_2As_2$", Journal of the Physical Society of Japan **79** (2010) 014714

(6) A.Q.R. Baron, "Status of the RIKEN Quantum NanoDynamics Beamline (BL43LXU): The Next Generation for Inelastic X-Ray Scattering." SPring-8 Information Newsletter, **15**, (2010) 14-19

(7) H. Uchiyama, S. Tsutsui, A.Q.R. Baron**,** "Effects of anisotropic charge on transverse optical phonons in NiO: Inelastic x-ray scattering spectroscopy study." Physical Review B, **81**, (2010) 241103R
(8) T. Ichitsubo, W. Itaka, E. Matsubara, H. Kato, S. Biwa, S. Hosokawa, K. Matsuda, J. Saida, O. Haruyama, Y. Yokoyama, H. Uchiyama and A.Q.R. Baron "Elastic inhomogeneity and acoustic phonons in Pd-, Pt-, and Zr-based metallic glasses." Physical Review B **81** (2010) 172201
(9) K. Yoshida, S. Hosokawa, A.Q.R**.** Baron and T. Yamaguchi, "Collective dynamics of hydrated β-lactogloblin by inelastic x-ray scattering." The Journal of Chemical Physics **133** (2010) 134501
(10) T. Sasagawa, H. Yui, S. Pyon, H. Takagi and A.Q.R. Baron "Phonon softening in $La_{1.74}Eu_{0.1}Sr_{0.16}CuO_4$ studied by inelastic X-ray scattering" Physica C **470** (2010) 551.

b. Oral Presentations

(1) A.Q.R. Baron, "Atomic Dynamics in Disordered Materials by Inelastic X-Ray Scattering", 66th Meeting of The Physical Society of Japan (Divisional Invited Talk), Japan, September 2010
(2) A.Q.R. Baron, "Recent Advances in meV-Resolution Measurements of Dynamics", Invited presentation at the 7th International Conference on Inelastic X-ray Scattering (IXS2010), Grenoble, France, October, 2010.
(3) A.Q.R. Baron, "Investigating meV Dynamics with X-Rays at SPring-8: Good, Bad, Recent, Future" Seminar at the Spallation Neutron Source (SNS), Oak Ridge, Tennessee, November 2010
(4) A.Q.R. Baron, "Phonons in $PrFeAsO_{1-x}$ by High Resolution Inelastic X-Ray Scattering", Invited presentation at the 9th International Conference Materials and Mechanisms of Superconductivity (M^2S 2009), Tokyo, Japan, September 2009
(5) A.Q.R. Baron, "meV-Resolution IXS: Recent Results and Future Prospects", Invited presentation at the Asia-Oceanic Forum on Synchrotron Radiation, Melbourne, Australia, December 2008

G. Future Plan

For the immediate future, MDL will continue construction and commissioning of BL43LXU. While the level of work required to match and, indeed, to move beyond the existing BL35 is large, especially given the desired short time scale, the increased number of channels, and the new spectrometer design, we hope that by the spring of 2012, the beamline will be performing well enough to begin first experiments. Initial scientific targets (among many) include (1) observation and investigation of orbiton dispersion, where the orbiton is the expected, but as yet unproven, excitation corresponding to orbital ordering of materials, and (2) investigations of temperature and doping dependence of weak phonon modes in cuprates. The recent large temperature dependence of the phonons observed in one cuprate (mentioned above) makes it very interesting to perform detailed investigations with respect to temperature (and momentum and energy transfer) to see the effect of the pseudo-gap and the superconducting gap on the phonon spectra. Another longer-term target of the electronic excitation work is direct investigation of low-energy gaps in electronic structure. The superconducting gap, for example, should be visible using IXS, somewhat similarly to Raman scattering. Such experiments are interesting as they should give a new probe of the gap symmetry, which remains a contentious issue in many materials. There are several additional directions for work, including those mentioned above (high pressure, surface scattering, multiferroics), and liquids dynamics, that will also continue at the new beamline and at BL35.

H. Curriculum Vitae (Associate Chief Scientist)

NAME: Alfred Q.R. Baron

DATE OF BIRTH: May 31, 1965, New York, USA

EDUCATION:

1995: Ph.D., Stanford University, Department of Applied Physics.
1988: B.S. Physics and B.A. Mathematics, High Honors, ΦBK,
Michigan State University.

DEGREES:

Ph.D. Applied Physics
B.S. Physics
B.A. Mathematics

RESEARCH APPOINTMENTS:

2006-: Associate Chief Scientist & Laboratory Head
Materials Dynamics Laboratory, SPring-8 Center, RIKEN
1997-: Japan Synchrotron Radiation Research Institute (JASRI)
Research and Utilization Division & Optics Group
Present Position: Senior Scientist and IXS Team Leader
1997-: Visiting Scientist, Coherent X-Ray Optics Laboratory, RIKEN
1997: European Synchrotron Radiation Facility (ESRF), Scientist
1995-1997: European Synchrotron Radiation Facility (ESRF), Post-Doc

ACADEMIC ACTIVITIES:

Membership
American Physical Society
Physical Society of Japan
Advisory Appointments
NSLS-II Experimental Facilities Advisory Council (EFAC) (2007-2009)
NSLS-II IXS Beamline Advisory Team (BAT) (2009-)
J-PARC Instrument Program Review Subcommittee (2008-)

2-5. Biostructural Mechanism Laboratory / 米倉生体機構研究室

Associate Chief Scientist; Koji YONEKURA, Ph. D. / 米倉 功治
Since Feb 2008

A. Research Topics (Highlights)

1. Structural study of ion-coupled energizing membrane proteins in bacteria

There are many essential biological processes coupled to ion potentials across the membrane. In *E. coli* or *Salmonella*, an inner membrane complex MotAB converts proton flux into rotation of the flagellum, enabling bacterial motility. There are other channel complexes that have weak sequence homology to MotAB, called ExbBD and TolQR. Although these homologs both utilize the ion motive force, they have very different physiological functions. ExbBD is involved in active transport of iron siderophore and vitamin B_{12} through the outer membrane, while TolQR is known to maintain the integrity of the outer membrane. We are aiming to analyze the structures of these complexes and elucidate the mechanism of the energy conversion system by X-ray crystallography and electron microscopy (EM). We have shown the first three-dimensional structure of this family by EM single particle analysis from mono-dispersed particles, and are now trying to make crystals to analyze their higher-resolution structures by X-ray and electron crystallography.

2. Structure analysis of telomere complexes

Telomere, which exists at the ends of eukaryotic chromosomes, is essential for faithful chromosome maintenance. Telomere length is regulated by proteins forming complexes with the telomeric DNA. Rap1 in *Saccharomyces cerevisiae* binds the telomeric repeats, and its C-terminus of Rap1 interacts with Rif1 and Rif2. To understand how these proteins regulate telomere length, we are studying the structures of these complexes by EM. Single particle electron tomography (ET) has revealed heterogeneous complexes, where one to twenty Rap1 molecules assemble in tandem and form various super structures. We are now carrying out cryo-EM and cryo-ET to analyze the structures of those complexes in a native stats or a state close to it.

3. Electron crystallography of tiny and thin three-dimensional crystals of biological macromolecules

Membrane proteins or macromolecular complexes often give tiny and thin crystals that are smaller than a few μm and thinner than 0.1 μm. Such samples are generally difficult to be obtained enough for many crystallization trials to grow to a suitable size for X-ray crystallography. Crystals with these dimensions often diffract electrons to higher than 2 Å resolution, because the scattering power of light atoms for electron is more than ~100,000 times higher than that for X-ray. X-rays scatter by electrons around atoms, while electrons scatter by coulomb potential of atoms. Hence it would be possible to observe experimental charge distributions of molecules, which will unravel the working mechanisms of biological nano-machines in detail. We have been developing a new method to analyze such tiny and thin protein crystal structures by cryo-EM.

4. Correlative imaging of biological complexes by electron microscopy and coherent X-ray diffraction microscopy

Cryo-EM is a suitable method to analyze the structures from various forms of biological

samples. Many techniques developed for cryo-EM can also be applied to coherent X-ray diffractive imaging (CXDI). CXDI is especially powerful for thicker samples such as whole cells and cell organelles. The high penetrating power can image such specimens without thin sectioning. It is, however, not an easy task to position a target of interest correctly for X-ray exposure since no real images are available. A correlative approach with cryo-EM is particularly useful; it can precheck sample conditions and produce a navigation map, which helps place the target in the right position. Also, cryo-EM can give initial phases for phase retrieval from poorer speckle patterns, which are typical of biological specimens. In collaboration with Prof. Nakasako's group of Keio University, we are working for correlative imaging with EM and coherent X-ray diffraction microscopy (CXDM). It includes the development of a new cryo-specimen holder, which can be used both with EM and CXDM.

B. Research Subjects

(1) Structural analysis of ion-coupled energizing membrane proteins in bacteria
(2) Structure analysis of telomere complexes
(3) Electron crystallography of tiny and thin three-dimensional crystals of biological macromolecules
(4) Correlative imaging of biological complexes by electron microscopy and coherent X-ray diffraction microscopy

C. Projects

Project name	Category	Started	Completed
Structural study of the torque-generating unit in the bacterial flagellar motor	MEXT, Grant-in-Aid for Scientific Research (B)	2008	2012
Development of a new cryo-specimen holder to study the structures of biological macromolecular complexes such as telomere by electron microscopy	Institute Program	2009	2009
Software development for electron crystallography of three-dimensional crystals of biological macromolecules	JST, Development of Advanced Measurement and Analysis Systems	2009	2011
Study for correlative imaging of biological complexes by electron microscopy and coherent X-ray diffraction microscopy	Institute Program	2010	2011

D. Members

as of March 1st, 2011

	number	Name
Research Scientist	2	Koji Yonekura, Masahiro Watanabe
Technical Scientist	0	
Research Staff	1	Yuko Kageyama
Technical Staff	0	
Visiting Researchers	0	
Trainees	0	

E. Funding

(million yen)

	FY2008	FY2009	FY2010
Laboratory budget from RIKEN	36	17	16
Competitive fund in RIKEN	1	23	10
Competitive fund outside RIKEN	8	5	9
Other fund from University, Private foundations etc.	0	0	0

F. Research Output

	FY2008	FY2009	FY2010
International Publications	2	1	1
Publications in Japanese	0	1	1
Oral Presentations	5	11	9
Patent Applications	0	0	0

a. Papers

(1) Maki-Yonekura S., and Yonekura K. : “Electron digital imaging towards high-resolution structure analysis of biological macromolecules”, Microsc. Microanal. 14, 362 - 369 (2008)

(2) Iwasaki K., Miyazaki N., Hammar L., Zhu Y., Omura T., Wu B., Sjöborg F., Yonekura K., Murata K., Namba K., Caspar D.L., Fujiyoshi Y., and Cheng R.H. : “Pleomorphic configuration of the trimeric capsid proteins of Rice dwarf virus that allows formation of both the outer capsid and tubular crystals”, J. Mol. Biol. 383, 252 - 265 (2008)

(3) Maki-Yonekura, S., Yonekura, K., and Namba, K. : “Conformational change of flagellin for polymorphic supercoiling of the flagellar filament”, Nat. Struct. Mol. Biol. 17, 417 - 422 (2010)

(4) Williams, T. L., Levy, D. L., Maki-Yonekura, S., Yonekura, K., and Blackburn, E. H. : “Characterization of the yeast telomere nucleoprotein core: Rap1 binds independently to each recognition site”, J. Biol. Chem. 285, 35814 - 35824 (2010)

(5) Yonekura K. : “Cryo-electron microscopy of biological macromolecular structures”, J. Crystallogr. Soc. Jpn 52, 56 - 61 (2010)

(6) Yonekura K. : “Electron imaging towards high-resolution structure analysis of biological macromolecules”, Microscopy, 45 243 - 249 (2010)

b. Oral Presentations (* Invited presentation)

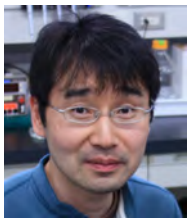
(1) Yonekura K. : “Cryo-electron microscopy of biological macromolecular structures”, Symposium “Present status and future prospect of microscopy by leading young Asian researchers”, The 66th annual meeting of the Japanese society of microscopy, Kyoto, Japan, May (2008)*
(2) Yonekura K., and Maki-Yonekura S. : “Cryo-electron microscopy of biological macromolecular structures”, The workshop on FEL science, Jeju, Korea, Feb. (2009)*
(3) Yonekura K., and Maki-Yonekura S. : “High-resolution cryo-electron microscopy of biological macromolecular structures by helical reconstruction”, Microscopy Conference 2009 in Graz, Graz, Austria, Sep. (2009)*
(4) Yonekura K. : “Cryo-electron microscopy of biological macromolecular structures”, SEMINAIRE IBS, Grenoble, France, Sep. (2009)*
(5) Yonekura K., and Maki-Yonekura S. : “Bioimaging---cryo-electron microscopy”, The second workshop on FEL science: “Emerging X-ray applications in biological systems”, Kenting, Taiwan, Dec. (2009)*
(6) Maki-Yonekura S., and Yonekura K. : “Cryo-electron microscopy and helical image reconstruction of biological materials”, Symposium leading young Asian researchers, The 66th annual meeting of the Japanese society of microscopy, Nagoya, Japan, May (2010)*
(7) Yonekura K., and Maki-Yonekura S.: “Correlative imaging --- CXDI and cryo-EM ---”, The 3rd Workshop on FEL Science: "Emerging X-ray applications in biological systems−II", Hokkaido, Japan, Oct. (2010)*
(8) Yonekura K. : “Electron crystallography in biological sciences”, The satellite meeting, The 10th conference of the Asian crystallographic association, Daejeon, Korea, Oct. (2010)*
(9) Yonekura K., and Maki-Yonekura S. : “Cryo-electron microscopy of biological macromolecular structures”, OIST seminar, Okinawa, Japan, Jan. (2011)*
(10) Yonekura K., and Maki-Yonekura S.: “Cryo-electron microscopy of biological macromolecules”, Workshop on structural biology, Tainan, Taiwan, Feb. (2011)*

G. Future Plan

There are many huge macromolecular complexes in living organisms, but these are often hard to crystallize because of their size, complexity and heterogeneity. Cryo-EM is a suitable method to analyze complex structures, because it can be applied to various forms of samples, e.g. two-dimensional crystal, helical assembly, spherical virus, dispersed particle, cell organelle and cell, although attainable resolution depends on the system. To extend this potential to higher resolutions, we have been devising various image analysis techniques for helical reconstruction, single particle analysis and cryo-ET. We will continue this effort particularly for electron crystallography of thin three-dimensional crystals. Also with our newly developed specimen holder, we will purse higher-resolution cryo-ET and correlative imaging with CXDM.

Our targets include ion-coupled energizing membrane proteins in bacteria, telomere and the bacterial flagellar motor. We will also use X-ray crystallography and CXDI by X-ray free electron laser to elucidate the working mechanisms of biological macromolecules in detail. For this purpose, we are working together with researchers inside and outside RIKEN SPring-8 Center.

H. Curriculum Vitae (Associate Chief Scientist)



NAME: Koji YONEKURA

DATE OF BIRTH: May 5, 1969

EDUCATION:

1992: Graduated from Tokyo Institute of Technology
1997: Master Degree from Graduate School of Biosciences, Tokyo Institute of Technology
1997: Ph. D. from Graduate School of Biosciences, Tokyo Institute of Technology

ACADEMIC DEGREES: Ph. D. (Structural biology)

APPOINTMENTS:

1997 : Research Associate, International Institute for Advanced Research, Matsushita Electric Company
1997-2000: Researcher, Protonic NanoMachine Project, ERATO, JST
2000-2002: Group Leader of NanoSwitching Group, Protonic NanoMachine Project, ERATO, JST
2002-2005: Assistant Professor, Graduate School of Frontier Biosciences, Osaka University
2004-2008: Keck Fellow, The W. M. Keck Advanced Microscopy Laboratory, Department of Biochemistry & Biophysics, University of California, San Francisco
2008- : Associate Chief Scientist, Biostructural Mechanism Laboratory, RIKEN SPring-8 Center
2008- : Lecturer (non-full time), Institute of molecular and cellular biosciences, The University of Tokyo

ACADEMIC ACTIVITIES:

2004-2008: Keck Fellow, The W. M. Keck Advanced Microscopy Laboratory
2009: The Ernst Ruska Prize of the German Society for Electron Microscopy

Membership

The Biophysical Society of Japan
2010-: Member of the specialty committee
The Japanese Society of Microscopy
2009-: Member of the younger generation subcommittee

2-6. Structural Physiology Research Group / 構造生理学研究グループ

Group Director; Atsuo MIYAZAWA, Dr. Sci. / 宮澤 淳夫
Since April 2006

A. Outline of the Research Group

Structural Physiology Research Group was established in April 2006 as 7-year-term project at RIKEN SPring-8 Center (RSC), consisting of the following 4 research teams, "Bio-multisome Research Team", "Three-dimensional Microscopy Research Team", "Molecular Signaling Research Team", and "X-ray Structural Analysis Research Team". The concept and construction of Structural Physiology Research Group is to shape the project according to the mission of RSC. For the field of life science, it appears that the most important mission of RSC should be to explore, promote and lead research utilizing unique and advanced synchrotron radiation related facilities at SPring-8. The research group is also designed so that the equipments and facilities, the laboratory space and the fund are shared by all 4 research teams. This is not simply for the efficient use of the research resources but more for encouraging frequent scientific discussions and sharing techniques and knowledge within the research group.

The study of research group is mainly to develop the basic technologies enabled the analysis of unclarified targets which are important for the understanding of the life function, by use of SPring-8, microscopies, and XFEL. It can be expected that the measurement that uses the highest performance light source generated by SPring-8 and XFEL, enables the structure analysis on the research object which could not be analyzed by current structural biological technique, and can greatly promote the answering and understanding of biological and physiological problems which has not been elucidated yet. On the other hand, it should be necessary to develop the proper strategy of sample preparation, measurement, and analytical method for the use of these novel equipments. Especially, the key point for the analysis of difficult object in the biological field is how to prepare specimens which can maintain the physiological function and endure the beam irradiation during the experimental procedure of structural analysis. Then, the each research in the research group is focused on analyzing the molecular structure and function of synapse, as the common platform among 4 research teams. Synapse is the most important place for cell-to-cell signaling, and where a lot of difficult research targets are still remained to be analyzed by structural biology. The 4 research teams in the research group coordinate on developing the modern basic technologies for the analysis of molecules, and the following experimental studies are advanced as described below briefly and in detail on the following pages of each research team.

Both Molecular Signaling Research Team and X-ray Structural Analysis Research Team investigate in the advanced strategy of X-ray crystallography using SPring-8. The Molecular Signaling Research Team contends with the structural analysis of transporter and sensory receptors, by developing unique preparations methods for crystallization of membrane proteins, which is the most difficult part in structural biology. The X-ray Structural Analysis Research Team makes serious efforts spending quite a long time on the analysis of the molecular dynamics of actin filament by progressive X-ray fiber diffraction approaches. On the other hand, both Bio-multisome Research Team and Three-dimensional Microscopy Research Team investigate in the structural and functional analysis of membrane protein complexes by the combination of electron microscopy and X-ray crystallography. At present, 3-dimensional analysis by electron microscopy, such as electron crystallography, single particle analysis, and electron tomography, are developing rapidly in the world and thought to

be greatly promising techniques, which are considered as complementary approaches to the study conducted by both SPring-8 and XFEL installed in Harima Institute.

By the end of the project, the 4 research teams will be able to conduct the study in accordance with the mission of RSC as the center of excellence for high-energy photon science, not only developing innovative techniques in X-ray crystallography related SPring-8, but also making new interdisciplinary fields in photon science among microscopies, SPring-8 and XFEL.

B. Response to the Midterm Review Report of the Research Group

All member of the Structural Physiology Research Group would like to appreciate reviewers' kind efforts to assess at interim research activities of the research group and also their inspiring comments on our 7-year-term project. Almost all comments for the research group are not only precise and to the point, but also helpful for the management of the projects as a research activity under the mission of RSC.

The reviewers mainly suggest the 2 points to improve the activity of the research group. One is the cooperation of the 4 research teams, and the other is the management of basic budget for the research group from RIKEN. About the cooperation of the 4 research teams, the reviewers described as following. "The 4 research teams works independently, and the research group looks an assembly of university laboratories. The coordination of the efforts by the 4 teams may be further improved. There will be the necessity to exhibit the results as the group whose term was limited. More cohesive efforts by the 4 team leaders towards more highly integrated research projects would be appreciated." We agree that our collaboration of 4 research teams could be more improved to have synergy effects in a specifically focused project. The study of the research group has been focused on analyzing the molecular structure and function of proteins closely related to signal transduction. According with reviewers' comments, we would like to more concentrate our efforts on well focused targets in the second half of the 7-year-term project. Secondly, the reviewers' comments suggest that the laboratory basic budget from RIKEN should be evenly distributed among the 4 research teams. We also agree, and we have already changed in the arrangement of how the financial resource should be distributed to allow each team to have more capacities in managing their own team's research activities.

One reviewer recommends that Bio-multisome Research Team should pay more attention to the RSC mission, and be better to collaborate more significantly to improve the activity. We are sure that Bio-multisome Research Team has been also paid more attention to the RSC mission and has plans to utilize effectively the synchrotron radiation and XFEL facilities. In the case of MEXT, Target Protein Research Program, the research team takes part in the structural analysis of bovine heart complex I by electron crystallography as well as X-ray crystallography at SPring-8, in collaboration with Prof. Yoshikawa at University of Hyogo and Dr. Aoyama at Osaka University. The team is also especially focusing in the aspects of microscopic utility of SPring-8, such as X-ray microscopy and X-ray microCT. The team has collaborated to reveal the 3 dimensional mapping of the brain of zebra fish. Furthermore, the study of the research team could contribute the development of imaging techniques for biological samples by XFEL. We think that the study of cryo-specimen preparation for cryo-electron microscopy might be useful for imaging by XFEL to observe the biological samples at a close to native state. And the development of genetically encoded protein tag using metal-binding proteins could be used for the identification of the biological molecules in the cell in the measurement of XFEL. The Bio-multisome Research Team has more accelerated to accept several collaborative studies utilizing the microscopic facilities in the

research group. The research team has started to do collaborative studies with more than 10 researchers after the midterm review of the group, as listed below. Electron tomography is being studied with Prof. Yasunaga at Kyushu Institute of Technology and Dr. Iwasaki at Osaka University. High pressure freezing is being studied with Dr. Noda at The University of Tokyo, Dr. Jinnai at Kyoto Institute of Technology, Dr. Morone at Kyoto University, Prof. Kuga at Hiroshima University, and Dr. Kotani at Nitto Analytical Techno Center. Cryo-electron microscopy is being studied with Dr. Kamei at Kyoto Insititute of Technology, Dr. Fujita at RIKEN Advanced Science Institute in Wako, and Dr. Shigemoto at Tokyo Metropolitan Institute of Gerontology. Dynamical X-ray observation of membrane protein using SPring-8 is being studied with Prof. Sasaki at The University of Tokyo. According with reviewers' comments, these collaborative researches could make it possible to activate and improve the activity of the research team. We shall do our best in the second half of the 7-year-term project, to obtain important results as many as possible.

C. Funding of the Research Group

(million yen)

	FY2008	FY2009	FY2010
Laboratory budget from RIKEN	16	12	19
Competitive fund in RIKEN	0	0	0
Competitive fund outside RIKEN	0	0	0
Other fund from University, Private foundations etc.	0	0	0

2-6-1. Bio-multisome Research Team / 生体マルチソーム研究チーム

Team Leader; Atsuo MIYAZAWA, Dr. Sci. / 宮澤 淳夫
Since April 2006

A. Research Topics (Highlights)

1. Two-dimensional crystallization of bovine heart Complex I

NADH-ubiquinone oxidoreductase (Complex I) is a main entry point of mitochondrial and bacterial respiratory chains. Complex I is one of the largest known membrane protein complexes. The molecular mass of bovine heart Complex I is about 1,000 kDa, containing at least 45 different subunits. To elucidate the structure of Complex I at high resolution by electron crystallography, Complex I was purified from bovine heart. As a result of extensive surveys, 2-dimensional crystals were obtained by dialysis with bovine heart phosphatidylcholine and cholesterol against a divalent cation-containing buffer. The obtained 2-dimensional crystals were next imaged in vitreous ice without any staining using a cryo-electron microscopy. The images of the ice embedded crystals did not show any arrays of protein molecules as seen in negatively stained images, but showed some diffraction spots as shown in Fig. 1.

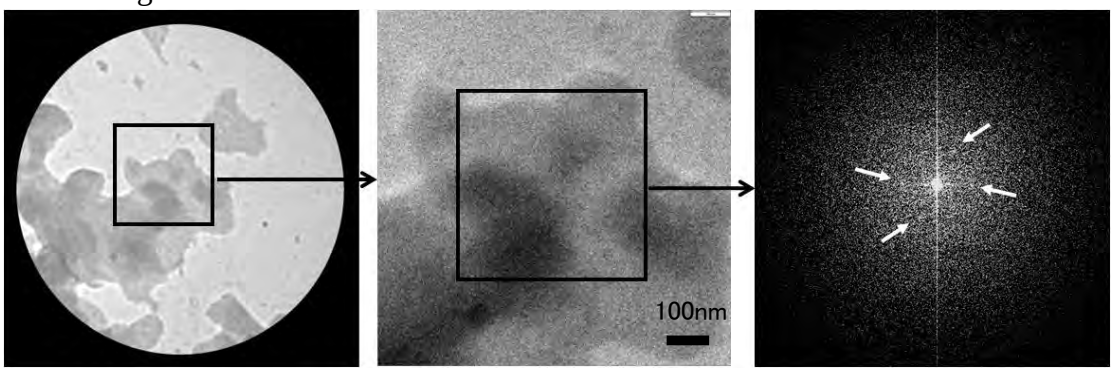


Fig. 1. Two-dimensional crystals of Complex I in vitreous ice. Two-dimensional crystals were imaged with a cryo-electron microscope x30,000 at 300 kV, and a fast Fourier transform was performed on the indicated box. The diffraction spots are indicated by arrows.

2. Observation of thick biological specimens by STEM tomography

Scanning transmission electron microscopy (STEM) tomography has not yet become popular in the field of biology. It is widely considered that the beam damage of STEM would be very severe, since a convergent electron beam is required for the imaging. On the other hand, STEM allows us taking tilt series of images from thick biological specimens (up to 1 μm) without using ultra-high voltage electron microscope for finding out 3-dimensional reconstruction of the specimens. Electron irradiation induced artificial structural changes which include the shrinkage of the resin in conventional biological specimen. These changes can be used as criteria for measuring the irradiation damage. To demonstrate an advantage of STEM tomography for the analysis of biological specimens, the shrinkage of the specimens was measured for the quantification of the beam irradiation-induced damage. Thick sections of resin-embedded HEK293 cells were used for the experiments. In the experiment for quantitative comparison, the electron dose used for transmission electron microscopy (TEM) and STEM imaging was identical. From table 1, it is clear that the shrinkage caused by STEM tomography was considerably less than that caused by TEM. The intensity of the beam must be high since the electron beam was convergent. However, the irradiation duration was very

short for a given point on the specimen that was being scanned. Intermittent and short irradiation was considered to facilitate the reduction of irradiation damage. Moreover, the probe size in STEM was approximately 0.6–1.0 nm, which was smaller than pixel size. It might be thought that the small probe size also aided in damage reduction.

Table 1 ‘after image’ / ‘before image’ rate

	A/B rate			
	Exp.1	Exp.2	Exp.3	Exp.4
Condition 1 (TEM, 3,500 electrons/pixel/sec,1 sec)	0.913 (–8.7%)	0.920 (–8.0%)	0.920 (–8.0%)	0.921 (–7.9%)
Condition 2 (TEM, 233 electrons/pixel/sec,15 sec)	0.940 (–6.0%)	0.947 (–5.3%)	0.935 (–6.5%)	
Condition 3 (STEM, 233 electrons/pixel/sec,15 sec)	1.000 (0%)	0.993 (–0.7%)	0.994 (–0.6%)	0.991 (–0.9%)

The shrinkage rates during data collection for electron tomography are shown. ‘before image’ was captured before obtaining the tomograsphy data. ‘after image’ was captured after obtaining the tomography data. The shrinkage rate is considered one of the criteria for the estimation of irradiation damage.

In this study, we applied STEM tomography to HEK293 cells and primary culture neurons. These cells, which were embedded in a resin, were cut into 1-μm-thick sections. Fig. 2 shows the 3-dimensional reconstructed structures of the cytoplasmic space of the HEK293 cell, as obtained by STEM tomography. In the 3-dimensional reconstructed images made from 1-μm-thick sections, it appears that the intra-cytoplasmic mitochondria fuse and form large reticular conformations in the cell. It has been previously confirmed by fluorescence microscopy that mitochondria form dynamic reticular networks maintained by a balanced frequency of fission and fusion events.

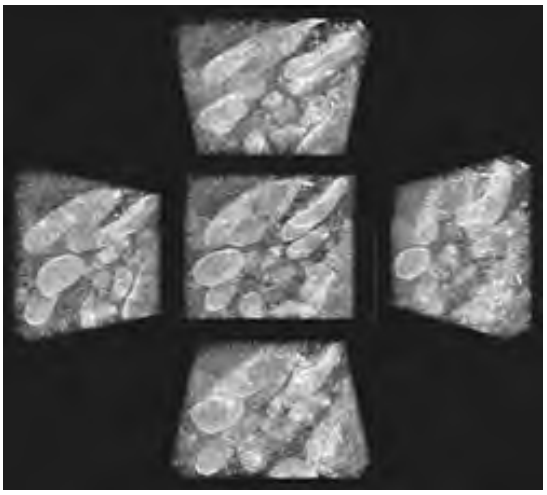


Fig. 2. Reconstructed 3-dimensional volume of HEK 293 cells. Volume-rendered image from various angles.

3. Application of 3MT-tag to CEMOVIS

Cryo-electron tomography is the most suitable method for exploring the 3-dimensional organization of biological samples with close-to-native preservation because this method involves a minimum of preparation-associated artifacts. However, conventional electron staining and immune-gold labeling are not available for the cryo specimens. Then, we have been developing the new technique of molecular labeling using genetically encoded tags of metal-binding proteins. Previously, we demonstrated that three tandem repeats of metallothionein (3MT) coordinating Cd^{2+} is a valuable genetically encoded tag to study the localization of the protein in cells by transmission electron microscopy with use of scaffold postsynaptic density-95 (PSD-95) coupled to 3MT (PSD-95-3MT) expressed in cultured hippocampal neurons (Fukunaga et al., J. Electron Microsc., 56, 119-129 (2007)). So as the next step, we aimed at applying 3MT tag to CEMOVIS (cryo-electron microscopy of vitreous sections). Because there was no precedent for obtaining cryo-sections of primary cultured neurons, we devised the method to make vitreous sections of primary cultured neurons. The neurons cultured in 3.5cm dishes were suspended in an artificial cerebrospinal fluid (ACSF) containing 124 mM NaCl, 1.2 mM KCl, 2.5 mM $CaCl_2$, 1.5 mM $MgCl_2$, 24 mM $NaHCO_3$,1.2

mM KH_2PO_4, 10 mM glucose, and 2 mM ascorbic acid at pH 7.4, supplemented with 20% dextran and 5% sucrose (w/v) acting as cryoprotectant. After freezing, the vitreous samples were trimmed and cryo-sectioned at -160°C. In the vitreous sections, membranes are well preserved and tubulins of a microtubule are found. And also, we found synapses characterized by synaptic vesicles. In future, to determine whether our genetically encoded tag (3MT-Cd) is detectable within cryo-sections, we are going to observe cryo-sections of primary cultured neurons transduced with PSD-95-3MT and incubated with $CdCl_2$.

4. Examination of metal for molecular labeling for electron microscopy

Until now, we developed 3MT tag coordinating Cd^{2+} that allows for efficient protein detection by transmission electron microscopy. The multimer of tagged proteins is discernible, however, tagged monomer proteins are not sufficiently electron dense for detection. Therefore, we began to examine several metals, aiming to detect monomer protein by electron microscopy. We have evaluated four kinds of gold and nine kinds of platinum compounds. The cellular toxicities induced by these compounds were lower than that induced by $CdCl_2$. Then we have determined the intracellular amount of platinum in the cells which were treated with cisdiamminedichloroplatinum (II) (cisDDP) or transdiamminedichloroplatinum (II) (transDDP). CisDDP-treated cells had higher platinum content than trasDDP-treated cells, indicating that cisDDP is suitable for intracellular labeling of 3MT rather than transDDP. We also found that about 20 platinum atoms were incorporated into single 3MT-GFP by treating the purified Cd-3MT-GFP with cisDDP. Although 4 platinum atoms were also detected in single GFP molecule without 3MT tag, it is likely hard to detect 4 platinum atoms-cluster by electron microscopy. In the near future, we are analyzing single 3MT-GFP treated with cisDDP by electron microscopy.

B. Research Subjects

(1) Structural analysis of membrane proteins by electron crystallography
(2) Structural and functional study of the synapse by electron and light microscopy
(3) Development of genetically encoded protein tag for electron microscopy

C. Projects

Project name	Category	Started	Completed
Structural and functional study of the complex of acetylcholine receptor with rapsyn	MEXT, Grant-in-Aid for Scientific Research (B)	2005	2008
Biomolecular tomography with molecular labels in the cell	JST, CREST	2006	2008
Three-dimensional structural analysis at high resolution and functional analysis aspiring to elucidate of the whole picture of action mechanism of mitochondrial cellular respiration	MEXT, Target Protein Research Program	2007	2009

D. Members

as of March 1st, 2011

	number	Name
Research Scientist	2	Atsuo Miyazawa, Yuri Nishino,
Technical Scientist	0	
Research Staff	2	Ai Hirase, Ai Higashihara
Technical Staff	0	
Visiting Researchers	11	-
Trainees	11	-

E. Funding

(million yen)

	FY2008	FY2009	FY2010
Laboratory budget from RIKEN	12	10	9
Competitive fund in RIKEN	4	5	0
Competitive fund outside RIKEN	25	5	0
Other fund from University, Private foundations etc.	0	0	0

F. Research Output

	FY2008	FY2009	FY2010
International Publications	2	0	0
Publications in Japanese	1	2	2
Oral Presentations	8	3	3
Patent Applications	0	0	0

a. Papers

(1) Aoyama K. ,Takagi T. , Hirase A. , and Miyazawa A. :
"STEM tomography for thick biological specimens", Ultramicroscopy, 109, 70-80 (2008)
(2) Shigemoto K. ,Kubo S. ,Jie C. ,Hato N. ,Abe Y. ,Ueda N. ,Kobayashi H. ,Kameda K. ,Mominoki K. ,Miyazawa A. ,Ishigami A. ,Matsuda S. ,and Maruyama N. :
"Myasthenia gravis experimentally induced with muscle-specific kinase", Annals of the New York Academy of Sciences, 1132, 93-98 (2008)

b. Oral Presentations (* Invited presentation)

(1) Nishino Y. ,Yasunaga T. ,and Miyazawa A. : "A new protein labeling technique using genetically encoded metallothionein tag for electron microscopy", 9th Asia-Pacific Microscopy Conference, Jeju, Korea, Nov. (2008)
(2) Miyazawa A. : "Development of a genetically encoded metalloprotein rag enabling protein detection by electron microscopy", The 39th NIPS International Symposium “Frontiers of Biological Imaging -Synergy of the Advanced Techniques-”, Okazaki Conference Center, Okazaki, Japan, Nov. (2008)*
(3) Miyazawa A. : "Development of genetically encoded protein tags for electron microscopy",

Grobal COE International Synaposium -Structural Biology from atoms to tissues-, University of Hyogo, Hyogo, Japan, Mar. (2009)*

(4) Nishino Y. ,and Miyazawa A. : "A genetically encoded metallothionein-tag for electron microscopy", China-Japan 3D-EM Forum 2010, Beijing, China, Jan. (2010)

(5) Hirase A. ,and Miyazawa A. : "Application of a genetically encoded tag to the detection of intracellular proteins by electron microscopy", China-Japan 3D-EM Forum 2010, Beijing, China, Jan. (2010)*

G. Future Plan

The study of Bio-multisome Research Team is mainly going to focus on the structure and function of the membrane protein complex at the postsynapse. The synapse of peripheral tissues, neuromuscular junction, has been less studied in comparison with that of central nervous system. In the result, there are still lots of questions needing to be solved to understand how it works. At the postsynaptic membrane of neuromuscular junction, nAChR is expressed and forms complexes with rapsyn, MuSK, and other proteins in the cytoplasm. The structural aberration of nAChR and the disorder of the clustering formation cause neuromuscular diseases. And the dynamic remodeling of distribution and arrangement of these molecules are concerned in the regulation of the synaptic transmission. To understand the physiological functions of the postsynapse from molecular level, it becomes to be essential to clarify the overall structure, configuration and localization of the nAChR cluster in the cell at close to a native state, as well as the high resolution 3-dimensional structure of individual proteins isolated from the cells. Then, we will take the combination of the all microscopic approaches, including X-ray microscopy and X-ray microCT using SPring-8 as well as light and electron microscopy, for the study of the neuromuscular junction.

Recent advances in cryo-electron tomography have made it possible to obtain 3-dimensional images of subcellular components isolated from cells in a relatively native state. To analyze these tomograms, it is necessary to identify and isolate the structure of interest from cells. But conventional immuno-gold labeling cannot penetrate into thick sections to label efficiently target proteins, and is impossible to apply on frozen sections. Then, we have been developing the new technique of molecular labeling using genetically encoded tags of metal-binding proteins. The molecular labeling technique could provides an alternative approach to immuno-based labeling that may in the future become a valuable tool for electron microscopy. Until now we have observed the genetically encoded-tagged proteins in the ultrathin sections. Coincidentally novel development of the rapid freezing technique for biological specimens makes it possible to see the biomolecular structure in the cells under the condition closer to the living state. In the near future, we are going to apply the genetically encoded tags to CEMOVIS, freeze fracture replica technique and the cryo-scanning electron microscopy.

The several attempts of Bio-multisome Research Team could contribute the development of imaging techniques for biological samples by XFEL. The study of cryo-specimen preparation for cryo-electron microscopy might be useful for the imaging procedure by XFEL, to observe the biological samples at a close to native state. And the development of genetically encoded tags using metal-binding proteins could be utilized for the identification of the biological molecules in the cell in the measurement of XFEL. We would like to try and establish the methods to observe the localization, to make the identification, and to analyze the structure of the proteins labeled with the genetically encoded protein tags in the frozen-hydrated cells by the combinational approach of XFEL and all microscopies.

H. Curriculum Vitae (Team Leader)

NAME: Atsuo MIYAZAWA

DATE OF BIRTH: September 12th, 1964

EDUCATION:
1988: Department of Biology, School of Education, Waseda University
1990: Graduate School of Science and Engineering, Waseda University
1993: Graduate School of Science and Engineering, Waseda University

ACADEMIC DEGREES: Dr. Sci.

APPOINTMENTS:
1992: Assistant Professor, Advanced Research Center for Human Sciences, Waseda University
1993: Research Scientist, Protein Engineering Research Institute
1995: Staff Scientist/Visiting Scientist, MRC Laboratory of Molecular Biology, UK
1998: Senior Research Associate, International Institute for Advanced Research, Matsushita Electric Industrial Co., Ltd.
1999: Contract Researcher, Bio-multisome Research Team, RIKEN Harima Institute
2003: Team Leader, Bio-multisome Research Team, RIKEN Harima Institute
2006: Group Director, Structural Physiology Research Group, RIKEN SPring-8 Center
2009: Professor, Graduate School of Life Science, University of Hyogo

ACADEMIC ACTIVITIES:
1996-1998: Awardee, Long-term Fellowships of Human Frontier Science Program
2006- : Councilor, Japanese Society of Microscopy
2006- : Member of Steering Committee, The 169th committee on Diffraction Structural Biology, Japan Society for the Promotion of Science
2007- : Research Collaborator, NPO Integrated Imaging Research Support
2009- : Executive Editor, Journal of Electron Microscopy, Oxford University Press

2-6-2. Three-dimensional Microscopy Research Team / 三次元顕微鏡法研究チーム

Team Leader; Teruhisa HIRAI, Dr. Sci. / 平井　照久
Since August 2006

A. Research Topics (Highlights)

We are currently focused on the structural analysis of membrane transporters that belong to ligand-driven transporter families. One is MFS (Major Facilitator Superfamily) family and another is AE (Anion Exchanger) family. Members of both families are widely distributed in animals, plants, yeast and bacteria and transport various substrates. For example, one member of MFS, the vesicular monoamine transporter (VMAT) is known as mammalian neurotransmitter transporter. NDCBE, a member of AE family is expressed in human brain and is known to regulate pH of neurons by Na^+-driven Cl^-/HCO_3 exchange. Any single transporter of MFS or AE family is not solved for a full set of conformations yet. To understand the mechanism of transporters, appropriate methods including various spectroscopic techniques need to be applied besides crystallographic studies. Furthermore, we are planning to apply the method of electron tomography to figure out the overall transport system.

1. Structural analysis of human anion exchanger, AE1

AE1 (Anion exchanger 1, band 3) is the representative member of AE family and it is the most abundant membrane protein in human erythrocyte. Membrane domain of AE1 exchanges HCO_3^- and Cl^- (it is called "chloride shift") and the decrease of pH facilitates the release of O_2 from hemoglobin. We reconstructed 7.5-Å resolution map after processing non-tilted and tilted images of 2D crystals collected using cryo-electron microscope. We applied carbon sandwich method for sample preparation to reduce beam-induced specimen charging. AE1 is cross-linked with one of inhibitors, H_2DIDS (4,4-diisothiocyanatostilbene-2, 2'-disulfonic acid) that fixes AE1 as an outward-open conformation. The structure of AE1 gave us a new insight for the architecture of this transporter family.

2. Structural analysis of bacterial oxalate transporter, OxlT

OxlT (Oxalate Transporter) that belongs to MFS is an oxalate ($^-$OOC-COO$^-$) /formate ($HCOO^-$) antiporter found in anaerobic bacteria named *Oxalobacter Formigenes*. This bacterium can generate proton-motive force as a result of oxalate/formate exchange. So far, the "closed" structure of OxlT is solved at 6.5 Å by electron crystallography. After improving the monodispersity of purified protein we are now trying to improve the quality of 2D crystals and we are also trying to make 3D crystal of OxlT in parallel. We are also searching more stable homologs and we are testing monoclonal antibodies to improve crystallinity of OxlT.

3. Structural analysis of membrane structure by electron tomography

To understand the overall transport system it is necessary to analyze whole membrane structure because transporters are usually part of cascade structure in the membrane. Electron tomographic analysis is applied to synaptosome that contains protein complexes around the cleft between pre and post synapse. Because of low contrast image without fiducial markers, alignment was done using PROTOMO developed at Florida State University with careful inspection.

B. Research Subjects

(1) 2D and 3D crystallization of membrane proteins for electron and X-ray crystallography

(2) Analysis of structure and mechanism of transporters
(3) Structural analysis of membrane transport system by electron tomography

C. Projects

Project name	Category	Started	Completed
Fundamental technology development of protein structure analysis toward effective drug discovery project	NEDO Grant	2007	2012

D. Members

as of March 1st, 2011

	number	Name
Research Scientist	3	Teruhisa HIRAI, Yohei IKEDA, Tetsuya SHIMIZU
Technical Scientist	0	
Research Staff	0	
Technical Staff	2	Kazuko Agari, Natsumi Kitamura
Visiting Researchers	2	
Trainees	0	

E. Funding

(million yen)

	FY2008	FY2009	FY2010
Laboratory budget from RIKEN	7	5	9
Competitive fund in RIKEN	0	4	0
Competitive fund outside RIKEN	12	12	9
Other fund from University, Private foundations etc.	0	0	0

F. Research Output

	FY2008	FY2009	FY2010
International Publications	0	7	3
Publications in Japanese	1	0	0
Oral Presentations	3	4	4
Patent Applications	0	0	0

a. Papers

(1) Hirai T. and Subramaniam S.: "Protein conformational changes in the bacteriorhodopsin photocycle: comparison of findings from electron and X-ray crystallographic analyses", PLoS ONE 4, No. 6, e5769-1-e5769-16 (2009)
(2) Hirai T., Subramaniam S., and Lanyi J.: "Structural snapshots of conformational changes in a seven-helix membrane protein: lessons from bacteriorhodopsin", Curr. Opin. Struct. Biol. 19, No. 4, 433-439 (2009)

(3) Yamaguchi T, Fujii T, Abe Y, Hirai T, Kang D, Namba K, Hamasaki N, and Mitsuoka K.: "Helical reconstruction of the outward open band 3 membrane domain of human erythrocyte in tubular crystals" J. Struct. Biol. 169(3), 406-412 (2010)
(4) Yamaguchi T., Ikeda Y., Abe Y., Kang D., Hamasaki N., and Hirai T.: "Structure of membrane domain of human erythrocyte anion exchanger 1 revealed by electron crystallography" J. Mol. Biol. 397(1), 179-189 (2010)
(5) Hirai T., Hamasaki N., Yamaguchi T., and Ikeda Y. "Topology models of anion exchanger 1 that incorporate the anti-parallel V-shaped motifs found in the EM structure", Biochem. Cell Biol. (in press)
(6) Yamagishi A., Ikeda Y., Komura M., Koike H., Satoh K., Itoh S., and Shibata Y.: "Shallow sink in an antenna pigment system of photosystem I of a marine centric diatom, Chaetoceros gracilis, revealed by ultrafast fluorescence spectroscopy at 17K" J. Phys. Chem. B 114, 9031-9038 (2010)
(7) Ogawa, S., Saka, M., Yoshizaki, T., Shimizu, T., Okuno, T., and Miyair, K.: "Purification, characterization and amino acid sequence of endopolygalacturonases IVa and IVb from fungus *Stereum purpureum*" J. Appl. Glycosci. 56(4), 261-266 (2009)
(8) Ogawa S., Shimizu T., Kimura T., Utoh K., Okuno T., and Miyairi K.: "The pro-form of Stereum purpureum endopolygalacturonase I is inactivated by a pro-sequence in the C-terminal region" Biosci. Biotechnol. Biochem. 74(3), 558-62 (2010)
(9) Miyairi, K, Ogawa, S., Kimura, T., Shimizu, T., and Okuno, T.: "Auto-inactivation of Stereum purpureum Proendopolygalacturonase I by C-terminal 44 Amino Acid Residues" J. Appl. Glycosci. 57(2), 151-156 (2010)
(10)Hirai T.: "Structure and function of membrane transporter revealed by electron crystallography" Nano-Imaging, NTS, 376-384 (2008)

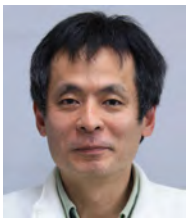
b. Oral Presentations (* Invited presentation)

(1) Hirai T.: "Structural analysis of macromolecule by electron microscopy", NIPS seminar, Okazaki, Sep. (2009)*
(2) Yamaguchi T.: "Helical image reconstruction of the membrane domain of human AE1 in tubular crystals", CSBMCB2010, Banff, Canada, Apr. (2010)*
(3) Hirai T.: "Structure of the membrane domain of human AE1 revealed by electron crystallography", CSBMCB2010, Banff, Canada, Apr. (2010)*
(4) Hirai T.: "Structure of erythrocyte membrane transporter AE1 solved by electron crystallography" JSM Xth Sectional Meeting on Structural Analysis of Biomaterial, Niigata, Dec. (2010)*

G. Future Plan

We used tube-like vesicular 2D crystals in both cases of OxlT and AE1 to obtain three-dimensional structure at moderate resolution (~6 Å). We are now focused on the sheet-like 2D crystal of which crystallinity is better than that of tube-like crystal. Besides improving the resolution, we also want to solve another conformations to explain whole conformational change of the transporter. For example, AE1 is known to take inward-open conformation with another inhibitor DEPC (diethypyrocarbonate). We think 2D crystal is a good target for XFEL (X-ray Free Electron Laser) in the near future. For cryo-electron crystallography, we only get one diffraction pattern from one 2D crystal at specific tilt axis and tilt angle because of electron beam damage. Even if we use XFEL as a beam source, severe beam damage will not require any additional work for us.

H. Curriculum Vitae (Team Leader)



NAME: Teruhisa HIRAI

DATE OF BIRTH: October 27, 1959

EDUCATION:

1984: Graduated from Department of Organic Chemistry, Faculty of Engineering, The University of Tokyo

ACADEMIC DEGREES:

1999: Dr. of Science from Department of Biophysics, Faculty of Science, Nagoya University

APPOINTMENTS:

1984-1990: Educational Staff, Digital Equipment Corporation, Tokyo, Japan
1990-1994: Research Scientist, Protein Engineering Research Institute, Osaka, Japan
1994-1999: Research Associate, International Institute for Advanced Research, Matsushita Electric Industrial Co., Ltd., Kyoto, Japan
1999-2000: Teaching Assistant, Department of Biophysics, Faculty of Science, Kyoto University, Japan
2000-2006: Research Fellow, Lab. of Cell Biology, NCI, NIH, Bethesda, MD, US
2006-2006: Staff Scientist, Lab. of Cell Biology, NCI, NIH, Bethesda, MD, US
2006-present: Team Leader at RIKEN Harima Institute, SPring-8 Center

ACADEMIC ACTIVITIES:

1999:Research Promotion Committee, Exploratory Research for Advanced Technology, Japan Science and Technology Corporation
1999: Kazato Research Award
2002: NIH FARE Award 2003
2003: HHS On-the-Spot Award

2-6-3. Molecular Signaling Research Team / 分子シグナリング研究チーム

Team Leader; Atsuko YAMASHITA, Dr. Agr. / 山下 敦子
Since April 2006

A. Research Topics (Highlights)

"Sense", such as vision, audition, touch sensation, gustation, and olfaction, is an important function for living organisms to receive, transduce, integrate, recognize and process a wide array of information from environment. We aim to elucidate molecular mechanisms of sensing processes through signal receptions from environment to signal transductions and transfers. The pivot of our study is structural analyses of proteins involving sensing, such as sensory receptors, signaling proteins, and ion channels, by X-ray crystallography using SPring-8 beamlines. Our target proteins include membrane proteins, which are currently one of the most important but challenging targets for structure analyses. Therefore, we have concurrently addressed the methodological development to facilitate membrane protein preparation and crystallization, in order to serve useful methods to the research filed of structural biology to make the most of SPring-8 beamlines. We also carry out functional analyses of the target proteins with biochemical and physiological approaches to understand the sensing mechanisms by integrating the structural and functional information.

1. Structural and functional analyses of sensory receptors

We have addressed structural analysis of yeast/fungus vacuole osmosensor channels as representatives of mechanosensory receptors. We newly identified a fungus osomosensitive cation channel, elucidated a region critical for the osomosensitive channel activity, and revealed the crystal structure of the region at 1.26 Å resolution. We performed mutation study based on the structural information, and revealed the structure basis for channel activity of this mechanosensitive receptor. Further functional analyses of the channel are in progress.

We have also addressed structural analyses of sweet/umami taste receptor as representatives of chemosensory receptors. After extensive screening of the samples and expression conditions, we established the conditions for large-scale production of taste receptors samples of the extracellular ligand binding domains by insect cell expression systems. The expressed samples turned out to be relatively unstable, but we found that the stabilizing conditions and established a purification process yielding samples with sufficient quality and quantity enough for crystallization. Some microcrystals have been obtained from the purified samples, and optimization of the crystallization conditions as well as sample preparation conditions are in progress.

2. Structural and functional analyses of signaling proteins in sensing systems

In order to grasp molecular process and the mechanisms of sensing comprehensively, we have addressed structure analyses of proteins involving in synaptic transmission, which link reception of external stimuli at sensory organs to signal transmission and recognition by the central nervous system. In collaboration with Prof. Matsuda at Kinki University and Prof. Okajima at Osaka university, we analyzed crystal structures of acetylcholine binding protein (AChBP), a soluble protein homologous to ligand binding domains of nicotinic acetylcholine receptors, in complex with various neonicotinoid insecticides. Different binding modes of the compounds were observed upon binding to the wild type AChBP and the AChBP mutants designed to mimic the receptors in insect nervous system, at least partly explaining various action modes of these insecticides to the receptors.

3. Research and development of methods to facilitate membrane protein crystallization

To lead successful crystallographic analyses of difficult target proteins including membrane proteins, we developed several new methods to facilitate the sample preparation and crystallization based on GFP-fusion techniques. We constructed a GFP-based screening system for insect cell expression, which is one of the most promising systems for eukaryotic membrane protein production. We confirmed that the system serves as a proper reporter for expression, localization, and folding of recombinant proteins within all expression spaces in the cells, such as the cytosol, organelles, and the extracellular space. We also established an improved native-PAGE method capable of evaluating the hydrodynamic states of membrane proteins and allowing in-gel fluorescence detection of tagged-GFP. The method achieved high-resolution electrophoretic separation in good agreement with the elution profiles analyzed by fluorescence-detection size-exclusion chromatography (FSEC), a useful technique for precrystallization screening, and might serve as a method for high-throughput precrystallization screening as well as a general analytical method for oligomerization or protein-complex formation for membrane proteins.

B. Research Subjects

(1) Structural and functional analyses of sensory receptors
(2) Structural and functional analyses of signaling proteins in sensing systems
(3) Research and development of methods to facilitate membrane protein crystallization

C. Projects

Project name	Category	Started	Completed
Crystallographic study for elucidation of functional mechanisms of sensory receptors	MEXT, Grant-in-Aid for Young Scientists (A)	2007	2009
Structural and functional analysis of taste receptors applicable to development of new taste substances and taste evaluation systems	MEXT, Target Protein Research Program	2007	2009
Development of innovative methods to support membrane protein crystallization	MEXT, Target Protein Research Program	2007	2009
Development of Advanced Production Technologies for Target Proteins	MEXT, Target Protein Research Program	2010	2010
Membrane transporters: structure and function of important drug targets	MEXT, Target Protein Research Program	2010	2010
Structure-biological elucidation of mechanisms of taste recognition by taste receptors	JSPS, Funding Program for Next Generation World-Leading Researchers	2010	2013

D. Members

as of March 1st, 2011

	number	Name
Research Scientist	3	Atsuko Yamashita, Makoto Ihara, Yuji Ashikawa,
Technical Scientist	0	
Research Staff	1	Noriko Matsuura
Technical Staff	0	
Visiting Researchers	0	
Trainees	2	

E. Funding

(million yen)

	FY2008	FY2009	FY2010
Laboratory budget from RIKEN	5	7	8
Competitive fund in RIKEN	1	1	0
Competitive fund outside RIKEN	37	32	23
Other fund from University, Private foundations etc.	0	0	0

F. Research Output

	FY2008	FY2009	FY2010
International Publications	3	1	3
Publications in Japanese	2	3	0
Oral Presentations	3	8	5
Patent Applications	0	0	0

a. Papers

(1) Ihara M., Matsuura N., and Yamashita A.: “High resolution Native-PAGE for membrane proteins capable of fluorescence detection and hydrodynamic-state evaluation", Anal. Biochem., 412, 217-223 (2011)

(2) Umeda T., Katsuki J., Ashikawa Y., Usami Y., Inoue K., Noguchi H., Fujimoto Z., Yamane H., and Nojiri H.: “Crystallization and preliminary X-ray diffraction studies of a terminal oxygenase of carbazole 1,9a-dioxygenase from Novosphingobium sp. KA1", Acta Cryst. F 66, 1480-1483 (2010)

(3) Umeda T., Katsuki J., Ashikawa Y., Usami Y., Inoue K., Noguchi H., Fujimoto Z., Yamane H., and Nojiri H.: “Crystallization and preliminary X-ray diffraction studies of a ferredoxin reductase component of carbazole 1,9a-dioxygenase from Novosphingobium sp.KA1", Acta Cryst. F **66**, 712-714 (2010).

(4) Inoue K., Ashikawa Y., Umeda T., Abo M., Katsuki J., Usami Y., Noguchi H., Fujimoto Z., Terada T., Yamane H., and Nojiri H.: “Specific interactions between the ferredoxin and terminal oxygenase components of a class IIB Rieske nonheme iron oxygenase, carbazole 1,9a-dioxygenase", J. Mol. Biol. **392**, 436-451 (2009)

(5) Singh S. K., Piscitelli C. L., Yamashita A., and Gouaux E.: “A Competitive Inhibitor Traps LeuT in an Open-to-Out Conformation", Science **322**, 1655-1661 (2008).

(6) Toshima K., Ihara M., Kanaoka S., Tarumoto K., Yamada A., Sattelle D. B., and Matsuda K.: “Potentiating and blocking actions of neonicotinoids on the response to acetylcholine of the neuronal α4β2 nicotinic acetylcholine receptor", J. Pesticide Sci. **33**, 146-151 (2008).

(7) Umeda T., Katsuki J., Usami Y., Inoue K., Noguchi H., Fujimoto Z., Ashikawa Y., Yamane H., and Nojiri H.: “Crystallization and preliminary X-ray diffraction studies of a novel ferredoxin involved in the dioxygenation ofcarbazole by Novosphingobium sp. KA1", Acta Cryst. F 64, 632-635 (2008)

b. Oral Presentations (* Invited presentation)

(1) Shimizu M., Goto M., Kawai T., Yamashita A., and Kusakabe Y.: “An Evaluation method for membrane trafficking of sweet taste receptor T1r2/T1r3", 8th International Symposium on Molecular and Neural Mechanisms of Taste and Olfactory Perception, Fukuoka, Nov. (2010).
(2) 山下敦子：“膜タンパク質のX線結晶構造解析：境界を超えて”,名古屋大学工学研究科・テクノシンポジウム「生物物理の未来研究会」,名古屋,9月(2010).*
(3) 山下敦子：“機能構造を保持した膜タンパク質の調製・結晶化・構造解析”,第10回日本蛋白質科学会年会,札幌,6月(2010).*
(4) Yamashita A., Singh S. K., Piscitelli C. L., and Gouaux E.: “Crystal structures of sodium-coupled transporter LeuT, a prokaryotic neurotransmitter transporter homolog, in the process of transport with its substrates or out of the process with its inhibitors", Innovative Nanoscience of Supermolecular Motor Proteins Working in Biomembranes, Kyoto, Sept. (2009).*
(5) 伊原誠：“ニコチン性アセチルコリン受容体に対するネオニコチノイド系殺虫剤の作用機構”,第270回細胞工学研究会,松江,4月(2008).*

G. Future Plan

The next subjects to be addressed is to link the mechanisms for the recognition of environmental signals, which are expected to be understood through the studies of our on-going projects, *i.e.*, the analyses of functional units of the sensory receptors, with the mechanisms of signal conversion or transduction into cellular signaling. To do this, structural information of the full-length receptors is crucial. We are therefore going to attempt structural analyses of the full-length sensory receptors. In addition, to understand how information from the environment is converted and relayed in the sensory signaling system, structural analyses of the receptors and signaling proteins in complex with proteins upstream or downstream of the signaling cascades are quite important and will also be our next targets for structural and functional studies. By integrating all of the structural and functional information we have gathered so far and will obtain in the future, we aim to understand the molecular mechanisms of the entire sensing system.

The full-length receptors and the protein complexes are difficult targets for structural analyses. The use of the high-brilliant X-ray beams from SPring-8, especially that with a very small focal size, is indispensable for the crystallographic structure determination of difficult targets. The X-ray beam from the XFEL facility with high coherency and intensity might also be useful for structural analyses of protein samples, their certain functional states, or certain protein complexes that are difficult to crystallize or just yields nanocrystals. However, conversely speaking, in order to make the best use of those powerful light sources, high-quality samples amenable to structural analyses are necessary. So far, we have developed several methods to facilitate membrane protein crystallization. We are continuing the methodological development to facilitate structural analyses of difficult target proteins, especially by focusing on protein preparation steps to yield high-quality samples. The developed methods are expected to enhance the successful structural analyses of difficult target proteins, including ours as sensory receptors, signaling proteins, and their complexes, using SPring-8 and XFEL facilities.

H. Curriculum Vitae (Team Leader)

NAME: Atsuko YAMASHITA

DATE OF BIRTH: December 29, 1970

EDUCATION:

1993: Graduated from Department of Agricultural Chemistry, Faculty of Agriculture, Kyoto University

1995: Master Degree from Division of Agricultural Chemistry, Graduate School of Agriculture, Kyoto University

1998: Ph. D. from Division of Agricultural Chemistry, Graduate School of Agriculture, Kyoto University

ACADEMIC DEGREES: Ph. D. (Agriculture), from Kyoto University

APPOINTMENTS:

1998-2000: Special Postdoctoral Researcher, RIKEN Harima Institute

2000-2006: Research Scientist, RIKEN Harima Institute

2003-2005: Concurrent Appointment of Postdoctoral Research Fellow, Columbia University

2006-present: Team Leader, RIKEN SPring-8 Center

2007: Concurrent Appointment of Visiting Lecturer, Graduate School of Pharmaceutical Sciences, Kyoto University

2008-present: Concurrent Appointment of Visiting Lecturer, School of Medicine, Keio University

ACADEMIC ACTIVITIES:

2009: The Young Scientists' Prize, The Commendation for Science and Technology by the Minister of Education, Culture, Sports, Science and Technology, Japan

2009-2010: Editorial Committee of “生物物理” (The Biophysical Society of Japan)

2010-present: Committee member, Astellas Foundation for Research on Metabolic Disorders

2010-present: Committee member, The Biophysical Society of Japan

2-6-4. X-ray Structural Analysis Research Team / X 線構造解析研究チーム

Team Leader; Toshiro Oda, Dr. sci /小田俊郎
Since April 2006

A. Research Topics (Highlights)

1. **Modeling for F-actin strcutre**
   Actin plays crucial parts in cell motility through a dynamic process driven by polymerization and depolymerization, that is, the globular (G) to fibrous (F) actin transition. Although our knowledge about the actin-based cellular functions and the molecules that regulate the G- to F-actin transition is growing, the structural aspects of the transition remain enigmatic. We created a model of F-actin using X-ray fibre diffraction intensities obtained from well oriented sols of rabbit skeletal muscle F-actin to 3.3 A in the radial direction and 5.6 A along the equator. Here we show that the G- to F-actin conformational transition is a simple relative rotation of the two major domains by about 20 degrees. As a result of the domain rotation, the actin molecule in the filament is flat. The flat form is essential for the formation of stable, helical F-actin. Our F-actin structure model provides the basis for understanding actin polymerization as well as its molecular interactions with actin-binding proteins. (Nature 2009)

2. **Dynamics of actin molecule…**
   Quasielastic neutron scattering (QENS) experiments were carried out on powders of F-actin and G-actin hydrated with D(2)O to characterize the internal dynamics on the picosecond time scale and the Ångstrom length scale. To investigate the effects of hydration, the measurements were done on samples at hydration ratio (h) of 0.4 (mg D(2)O/mg protein), containing only the first layer of hydration water, and at h = 1.0, containing more layers of water. The QENS spectra, obtained from the measurements at two energy resolutions of 110 and 15 μeV, indicated that the internal motions of both F-actin and G-actin have distributions of motions with distinct correlation times and amplitudes. Increasing hydration changes relative populations of these distinct motions. The effects of hydration were shown to be different between F-actin and G-actin. Elastic incoherent neutron scattering measurements provided the concerted results. The observed effects were interpreted in terms of the dynamical heterogeneity of the actin molecule: in G-actin, more surface loops become flexible and undergo diffusive motions of large amplitudes, whereas in F-actin the molecular interactions that keep the polymerized state suppress the large motions of the surface loops involved with polymerization so that the population of atoms undergoing large motions can increase only to a lesser degree. (Collaboration with Dr. Fujiwara in JAERI: Eour biophys J in press)

3. **Interaction of actin nucleation factor Spir with F-actin**
   Spire is an actin nucleator that initiates actin polymerization at a specific place in the cell. Similar to the Arp2/3 complex, spire was initially considered to bind to the pointed end of the actin filament when it generates a new actin filament. Subsequently, spire was reported to be associated with the barbed end (B-end); thus, there is still no consensus regarding the end with which spire interacts. Here, we report direct evidence that spire binds to the B-end of the actin filament, under conditions where spire accelerates actin polymerization. Using electron microscopy, we visualized the location of spire bound to

the filament by gold nanoparticle labeling of the histidine-tagged spire, and the polarity of the actin filament was determined by image analysis. In addition, our results suggest that multiple spires, linked through one gold nanoparticle, enhance the acceleration of actin polymerization. The B-end binding of spire provides the basis for understanding its functional mechanism in the cell. (JMB in press)

4. **Strcure of HLSV**
Hibiscus latent Singapore virus (HLSV) is a rigid rod-shaped plant virus and a new member of the Tobamovirus family. Unlike all other Tobamoviruses, the HLSV genome contains a unique poly(A) tract in its 3' untranslated region. The virion is composed of a monomeric coat protein (CP) unit of 18 kDa, arranged as a right-handed helix around the virus axis. We have determined the structure of HLSV at 3.5 Å by X-ray fiber diffraction and refined it to an R-factor of 0.096. While the overall structure of the HLSV CP resembles that of other Tobamoviruses, there are a few unique differences. There is a kink in the LR helix due to the presence of His122. Also, the adjacent Lys123 may further destabilize the helix by positive charge repulsion, making the kink more pronounced. The His122-Asp88 salt bridge provides significant stability to the loop adjacent to the RR helix. Carboxyl-carboxylate interactions that drive viral disassembly are also different in HLSV. The nucleotide recognition mechanisms for virus assembly between HLSV and ribgrass mosaic virus are similar, but different between tobacco mosaic virus and cucumber green mottle mosaic virus. (Collaboration with Prof.Swaminathana K in Singapole national university: JMB 406, 416-426 (2011))

B. Research Subjects

(1) Structure and dynamics of F-actin
(2) The initial process of actin polymerization and nucleation factors
(3) Actin function by the use of actin mutant
(4) Dvelopement of X-ray fiber diffraction analysis

C. Projects

Project name	Category	Started	Completed
A single molecule Pathology	MEXT, Grant-in-Aid for Scientific Research (C)	2009	2011
Development of instruments for the time-resolved X-ray small angle scattering	Institute Program	2009	2009

D. Members

as of March 1st, 2011

	number	Name
Research Scientist	2	Toshiro Oda, Tomoki Aihara
Technical Scientist	0	
Research Staff	0	

Technical Staff	0	
Visiting Researchers	1	
Trainees	0	

E. Funding

(million yen)

	FY2008	FY2009	FY2010
Laboratory budget from RIKEN	6	5	9
Competitive fund in RIKEN	0	8	0
Competitive fund outside RIKEN	0	0	0
Other fund from University, Private foundations etc.	0	0	0

F. Research Output

	FY2008	FY2009	FY2010
International Publications	4	5	4
Publications in Japanese	0	3	0
Oral Presentations	2	6	3
Patent Applications	0	0	0

a. Papers

(1) Popp D., Narita A., Oda T., Fujisawa T., Matsuo H., Nitanai Y., Iwasa M., Maeda K., Onishi H., and Maéda Y.: "Molecular structure of the ParM polymer and the mechanism leading to its nucleotide-driven dynamic instability", EMBO J 27, 570-579. (2008)

(2) Waldmann H., Hu T-S., Renner S., S. Menninger S., Tannert R., Oda T., and Arndt S-D.: "Total Synthesis of Chondramide C and its Binding Mode to F-Actin" Angew. Chem. Int. Ed. Engl. 47, 6473-6477. (2008)

(3) Fujiwara S., Plazanet M., Matsumoto F., and Oda T.: "Differences in internal dynamics of actin under different structural states detected by neutron scattering", Biophys. J. 94, 4880-4889. (2008)

(4) Iwasa M., Maeda K., Narita A., Maéda Y., and Oda T.: "Dual roles of Gln137 of actin revealed by recombinant human cardiac muscle alpha-actin mutants", J. Biol. Chem. 283, 21045-21053. (2008)

(5) Oda T., Iwasa M., Aihara T., Maéda Y., and Narita, A.: "The nature of the globular- to fibrous-actin transition" *Nature.* 457, 441-445. (2009)

(6) Popp D., Iwasa M., Maeda K., Narita A., Oda T., and Maéda Y.: "Protofilament formation of ParM mutants" *J. Mol. Biol.* 388: 209-217. (2009)

(7) Popp D., Iwasa M., Maeda K., Narita A., Oda T., and Maeda Y.: "Protofilament formation of ParM mutants", J. Mol. Biol. 388, 209–217 (2009).

(8) Machida Y. N., Kurosawa M., Nukina N., Ito K., Oda T., and Tanaka M.: "Distinct conformations of in vitro and in vivo amyloids of huntingtin-exon1 show different cytotoxicity", Proc. Natl. Acad. Sci. USA 106, 9679–9684 (2009).

(9) Splettstoesser T., Noe F., Oda T., and Smith J. C.: "Nucleotide-dependence of G-actin conformation from multiple molecular dynamics simulations and observation of a putatively polymerization-competent super- closed state", Proteins: Struct. Funct. Bioinf. 76, 353–364 (2009).

(10) Matsumoto F., Deshimaru S., Oda T., and Fujiwara S.: “Reconstitution of the muscle thin filament from recombinant troponin components and the native thin filaments”, Anal. Biochem. 399, 299–301 (2010).
(11) Matsuo T., Ueno Y., Takezawa Y., Sugimoto Y., Oda T., and Wakabayashi K.: “X-ray fiber diffraction modeling of structural changes of the thin filament upon activation of live vertebrate skeletal muscles”, Biophysics 6, 13–26 (2010).
(12) Popp D., Narita A., Ghoshdastider U., Maeda K., Maeda Y., Oda T., Fujisawa T., Onishi H., Ito K., and Robinson R. C.: “Polymeric structures and dynamic properties of the bacterial actin AlfA”, J. Mol. Biol. 397, 1031–1041 (2010).
(13) Tewarya S.K., Oda T., Kendall A., Bian W., Stubbs G., Wonga S.-M., and Swaminathana K.:, “Structure determination of Hibiscus latent Singapore virus by X-ray fiber diffraction: a non-conserved His122 contributes to coat protein stability.”, J Mol. Biol. 406, 416-426 (2011)
(14) Ito T, Hirayama T, Taki M, Iyoshi S, Dai S, Takeda S, Kimura-Sakiyama C, Oda T., Yamamoto Y, Maéda Y, and Narita A.: “ Electron Microscopic Visualization of the Filament Binding Mode of Actin-Binding Proteins”, J Mol Biol. (in press)
(15) Fujiwara S., Plazanet M., Matsumoto F.,and Oda T.: “Internal motions of actin characterized by quasielastic neutron scattering”, European Biophysics Journal (in press)
(16) Ito T., Narita A., Hirayama T,, Taki M., Iyoshi S., Yamamoto Y., Maéda Y., Oda T.: “Human Spire Interacts with the Barbed End of the Actin Filament.”, J Mol. Biol. (in press)
(17) A. Narita, T. Oda, Y. Maéda Cryo-electron microscopy revealed why the actin pointed end is the slow end. EMBO J (in press)

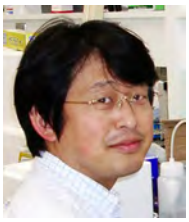
b. Oral Presentations (* Invited presentation)

（1） 小田俊郎 ”アクチンの構造とダイナミックス” 大阪大学蛋白質研究所セミナー「電子顕微鏡最先端」 大阪 2 月 (2011)*
（2） Oda T.: “Structure and Dynamics of actin molecule” IMCB seminar, Institute of molecular cell biology, Singapore (2010)*
（3） 小田俊郎 ”アクチンの構造とダイナミックス” 日本学術振興会 回折構造生物第 169 委員会 東京 11 月 (2010)*
（4） 小田俊郎 “重合にともなうアクチン分子の構造変化” 日本生物物理学会第 47 回年会シンポジウム 徳島 10 月 (2009)*
（5） 小田俊郎 “アクチン G-F 変換に伴う構造変化" シンポジウム：名大の生物物理の生誕 50 周年 名古屋 3 月 (2009)*
（6） 小田俊郎 “The nature of globular- to fibrous-actin transition” 阪大蛋白研蛋白質情報科学研究系セミナー 大阪 2 月 (2009)*
（7） Oda T.: “Novel Model for F-actin structure.” International Symposium “Thick and Thin Filament Regulation in Striated Muscle” Madison USA. April (2008)*

G. Future Plan

We develop the methodology for f0ber diffraction analysis of rod-like protein complex, and the simultaneous measurement apparatus of time resolved X-ray small angle scattering profies with flouresence signals, equipped with the rapid mixing instruments. Using these thechique, we study the dynamics and high resolution structure of F-actin, and formation of F-actin. Finally, we understand the mechanism of physiological events incuding actin dynamics, for example cell motuility, based on the fundermental function of actin molecule/

H. Curriculum Vitae (Team Leader)



NAME: Toshiro ODA

DATE OF BIRTH: August 10, 1964

EDUCATION:

1988: BS from Department of Physics, Facility of Science, Nagoya University
1990: MS from Department Physics, Facility of Science, Nagoya University
1995: PhD from Department of Physics, Facility of Science, Nagoya University

ACADEMIC DEGREES: Dr. Sci.

APPOINTMENTS:

1995-1999	Research Associate, International Institute Advanced Research (IIAR), Matsushita Electric Industrial Co. Ltd., Japan
1999-2004	Scientist, RIKEN Harima Institute, RIKEN SPring-8 center 2000-2002 Gust Scientist, Max-Planck Institute for medical research, Heidelberg, Germany
2004-2006	Senior Scientist, RIKEN Harima Institute, RIKEN SPring-8 center 2004-2008 Group Leader, ERATO Actin Filament Dynamics Project
2006-Present	Team Leader, RIKEN SPring-8 center

ACADEMIC ACTIVITIES:

The biophysical society of Japan

2. Photon Science Research Division

2-7. SR System Biology Research Group / 放射光システム生物学研究グループ

Group Director; Seiki KURAMITSU, Dr. Sci. / 倉光 成紀
Since April 2006

A. Outline of the Research Group

This research group is aiming at imaging from the “molecular level” to the “cellular level” of a single cell. To achieve this goal, we chose the extremely thermophilic organism, *Thermus thermophilus* HB8, as a model organism, because most of the 2,200 genes (proteins) encoded in its genome have been selected during evolution and are common to many organisms, including human. Furthermore, since its constituent molecules are thermostable and adequate for structural and functional analyses, this model organism is an excellent candidate for cellular and molecular imaging with the SPring-8 beamlines as well as X-ray structural analyses of its macromolecules.

In terms of the “molecular imaging”, about 22% of the total protein structures have been determined mainly by X-ray crystallography, and this model organism (*T. thermophilus* HB8) has become one of the most advanced organisms in genome-wide structural analysis (Structural Genomics).

In parallel to the structural analysis by conventional X-ray crystallography, the new proteins for future XFEL analysis were prepared.

1. Molecular Imaging (Structural Genomics) for Whole-Cell Imaging

For the whole-cell imaging at the atomic level, structural information for each molecule is necessary. Therefore, we determined as many protein structures as possible. The structures of over 22% of the total proteins (494 proteins) in this model organism have been determined, and this success rate for structural analysis is the highest among all organisms.

In addition to the single-molecule imaging, we are constructing a fixation system for single molecules, for future single-molecule imaging by XFEL.

2. Cellular Imaging

Cellular imaging has been performed by cryo-electron tomography and scanning X-ray fluorescence microscopy in collaboration with other groups.

In order to understand the cellular image, the functional information of each molecule is essential. Surprisingly, our genome analysis revealed that as many as 1/3 of the 2,200 total proteins (genes) are functionally uncharacterized, although many of them are essential and common to many organisms, including human. If we compare the situation for these functionally-uncharacterized proteins to "the periodic table of the elements", then the current situation corresponds to 1/3 of the periodic table being unknown. In order to interpret the whole-cell phenomena, the functionally-uncharacterized proteins must be identified. Therefore, we elucidated their functions (1) by using the structural data obtained from structural genomics as described above, and (2) by using the genome-wide functomics data obtained from mRNA analysis (transcriptomics), protein analysis (proteomics), and metabolite analysis (metabolomics), and then (3) we confirmed the function of each isolated protein *in vitro*.

3. Contributions to Research Communities, and Collaborations with Other Groups

The plasmids for protein expression (2,050 clones) and the plasmids for gene disruption (1,000 clones) prepared in our laboratory are available to the public through the RIKEN BioResource Center (see http://www.thermus.org/). Some of the information on protein production (protein expression and purification), crystallization, structure, and functomics (transcriptomics, proteomics, and metabolomics) is also available in the public databases. Our research group collaborates with many researchers at RIKEN, universities, and companies. We also host an annual meeting at SPring-8 every summer for exchanging information. More than one hundred researchers attend this meeting every year.

4. The Three Teams in This Research Group

This research group consists of three teams.

The “Functomics Integration Research Team” contributes mainly to the construction of resources, databases, and new research platforms, including preliminary analyses for future imagings. The subsystems used for developing these methods are DNA repair subsystems, which are related to “the central-dogma subsystems”. This team also contributes to the research groups in RIKEN and to the global research community. All of the members in the other teams (Functomics Biology I and II Research Teams) also contribute to the activities of the Functomics Integration Research Team.

The “Functomics Biology I Reseach Team (Team I)” is discovering the functions of the remaining 450 functionally-unknown proteins (genes), to understand the whole-cell image. For that purpose, Team I is analyzing the mRNA-synthesis (transcriptional network) subsystem, which is one of the “central-dogma subsystems”. Team I is also performing collaborative work for the whole-cell imaging by using the scanning X-ray fluorescence microscope at the BL29XU station.

The “Functomics Biology II Research Team (Team II)” is developing new molecular-imaging methods for analyzing multi-submolecular and dynamic complexes by using the pulse coherent X-ray of XFEL. For that purpose, Team II mainly uses protein-synthesis (translation) subsystem, which is also one of the “central-dogma subsystems”.

B. Funding of Research Group

(million yen)

	FY2008	FY2009	FY2010
Laboratory budget from RIKEN	43	43	42
Competitive fund in RIKEN	0	0	0
Competitive fund outside RIKEN	0	0	0
Other fund from University, Private foundations etc.	0	0	0

2-7-1. Functomics Integration Research Team / システム生物学統合研究チーム

Team Leader; Seiki Kuramitsu, Dr. Sci. / 倉光 成紀
Since April 2006

A. Research Topics (Highlights)

The minimum gene set estimated as being essential for a free-living organism is about 1,500. Microorganisms living in extreme environments often have about this number of genes, which are common to and indispensable for other organisms, including human. Understanding fundamental biological phenomena on the basis of the structures and the functions of biomolecules from one organism is essential to gain systems-level insight into organisms.

This research team contributes mainly to the construction of resources, databases, and new research platforms, including preliminary analyses for future imagings, and provides them to the other teams (Functomics Biology I and II Research Teams). This team also contributes by supplying resources to the research groups in RIKEN and to the global research community.

1. Protein Production for Molecular Imaging

1-1. Protein Production

Among the 2,200 total proteins encoded by the *T. thermophilus* HB8 genome, about 70% (1,500 proteins) were successfully overexpressed. Among these overexpressed proteins, 65% (970 proteins) were successfully purified. These purified proteins were used for system biological studies and molecular imaging at an atomic level. About 22% of the total protein structures have been determined mainly by X-ray crystallography, and this model organism has become one of the most advanced organisms in genome-wide structural analysis (structural genomics). This success rate for structural determination is the highest among all organisms.

Proteins for A Single-Molecule Imaging for Future XFEL

We found that some of the proteins in DNA repair subsystems strongly bound to a damaged base in DNA (Kosaka, H. *et al.* (2007) *J. Mol. Biol.* **373**, 839-850; Fukui, K. *et al.* (2008) *J. Biol. Chem.* **283**, 12136-12145). These DNA-repair proteins will be useful for fixing the target protein on the DNA in vacuo, because the proteins from *T. thermophilus* HB8 are known to be stable in vacuum conditions. Therefore, we constructed a new protein, with the DNA-binding domain on the N-terminal side and the target-protein domain on the C-terminal side. A His-tag was also attached to the C-terminus of the new protein. The target C-terminal domain in this new protein can be fixed by three points: two points by the DNA and one by the His-tag. This protein fixing system is being constructed in collaboration with Professor T. Yanagida, and will be useful for single-molecule imaging for future XFEL.

Membrane Protein Expression

The expression of the membrane proteins with 4 to 8 transmembrane helices were tried by using the *in vivo* expression system of *E. coli* with attaching the Mistic (membrane-integrating sequence for translation of integral membrane protein constructs) tag of *Bacillus subtilis* (Roosild, T. P. *et al.* (2005) *Science* **307**, 1317-1321) to their N-terminals. Twelve transmembrane proteins were tested for overproduction by the Mistic system, and eight of them were successfully expressed. This success rate of about 65% will be enough for the future membrane-protein project for structural and functional analysis.

Multi-subunit protein expression

To analyze multi-subunit protein complex, in vivo N-terminal and C-terminal His-tagging systems were constructed. These tagging systems and mass spectrometry provide the information for the components in the multi-subunit proteins. This information enables the coexpression of subunits of multisubunit proteins (for example, Nakai, T. *et al.* (2008) *J. Biochem.* **143**, 747-758).

2. Cellular Imaging

Single cell imaging *in vivo* was attempted by cryo-electron tomography in collaboration with Prof. K. Nagayama, and some vacuoles, fibers, and large molecules such as ribosomes were clearly identified. In order to understand the role of the particles (molecules) observed by cryo-electron tomography, functional identification of those molecules is essential. However, the functions of more than 500 protein molecules remained unknown. Therefore, we are systematically discovering their functions as described in the next section (**3. Developing New Platforms for Functional Analysis (Fuctomics)**).

Another mode of single cell imaging by metal ions was attempted, using scanning X-ray fluorescence microscopy at SPring-8 beamline BL29XU in collaboration with Drs. Yamauchi and Ishikawa's groups and with Team I. We found that most of the metal ions were bound to large molecules. Therefore, when the resolution of the cell imaging is increased, the bound metal ion in the large molecule will be structurally identified.

3. Developing New Platforms for Functional Analysis (Functomics)

The *T. thermophilus* HB8 genome has about 2,200 genes, and about 1/3 of the genes (proteins) are functionally unknown. These proteins are conserved in almost all organisms, ranging from bacteria to human. Functional analyses of these proteins are necessary to interpret the whole-cell imaging data.

Since the three-dimensional structure of a protein is more strictly conserved than the amino acid sequence during evolution, the structural information of a hypothetical protein can provide insight into its function. Our structural analyses yielded functional clues for about 60% of the proteins with solved structures. The success rate of structural determination was about 20%. Therefore, the functions of about 90% of the functionally-unknown proteins still remain to be discovered.

To determine the functions of these functionally-unknown proteins, genome-wide analyses by mRNA expression analysis (transcriptomics), proteomics analysis (proteomics), and metabolite analysis (metabolomics) were effective. This team constructed the platforms for these analyses, including the gene manipulating systems.

3-1. mRNA analysis (transcriptomics)

The GeneChip TTHB8401a520105F (revision 2) contains probe sets of 25-mer oligonucleotides representing 2,266 ORFs and their intergenic regions of the *T. thermophilus* genome. The platform for mRNA expression analysis (GEO accession no. GPL9209) has been constructed. We have designated protocols for DNA microarray analysis using the GeneChip. Our gene disruption system (Hashimoto, Y. *et al.* (2001) *FEBS Lett.* **506**, 231-234) is very useful to investigate the functions of genes by means of the DNA microarray analysis.

3-2. Protein expression analysis (proteomics)

Protein expression was analyzed with a Fourier-transform ion cyclotron resonance mass spectrometer (FT-ICR MS). The whole-cell proteins were analyzed as follows. (1) After cell lysis, whole proteins were digested with trypsin or lysylendopeptidase. (When the protein expression was compared between the two conditions, one sample is digested in the presence of $H_2{}^{16}O$, and another in the presence of $H_2{}^{18}O$.) (2) The peptides were separated by nano-liquid-chromatography (nano-LC) system, and followed by FT-ICR mass analysis. This

protein analyzing system identified more than 94% of the proteins. Therefore, it was found that most “hypothetical proteins” were expressed in the cell. Using this proteomics platform, it was also found that the expression profile of the proteins was quite different from that of mRNA.

3-3. Metabolite analysis (metabolomics)

Metabolites in the whole cell were also analyzed by mass spectrometry in collaboration with Professor M. Tomita of Keio University (Ooga, T. *et al.* (2009) *J. Biol. Chem.* **284**, 15449-15456).

4. Supporting research communities (supplying resources)

The plasmids for protein expression (2,050 clones) and the plasmids for gene disruption (1,000 clones) are available to the public through the RIKEN BioResource Center (see http://www.thermus.org). Some of the information about protein production (protein expression and purification), crystallization, structure, and functomics (transcriptomics, proteomics, and metabolomics) is also available from our database (http://www.thermus.org) and public databases. By using these resources, we have collaborated with many researchers at RIKEN, universities, and companies. We also exchanged our information in an annual meeting at SPring-8.

B. Research Subjects

(1) Systems biology of an extremely thermophilic model organism
(2) Molecular imaging
(3) Cellular imaging
(4) Functional discovery of new proteins
(5) Supplying resources

C. Projects

Project name	Category	Started	Completed
Structural and functional analysis of homologous recombination-suppressing system.	MEXT, Grants-in-Aid for Young Scientists (Start-up)	2008	2008

D. Members

as of March 1st, 2011

	number	Name
Research Scientist	1	Seiki Kuramitsu
Technical Scientist	0	
Research Staff	0	
Technical Staff	2	Kayoko Matsumoto, Toshi Arima,
Visiting Researchers	35	
Trainees	9	

E. Funding

(million yen)

	FY2008	FY2009	FY2010
Laboratory budget from RIKEN	3	2	2
Competitive fund in RIKEN	0	0	0
Competitive fund outside RIKEN	1	0	0
Other fund from University, Private foundations etc.	0	0	0

F. Research Output

	FY2008	FY2009	FY2010
International Publications	9	13	10
Publications in Japanese	1	1	0
Oral Presentations	56	38	39
Patent Applications	0	0	0

a. Papers

(1) Kondo, N., Nishikubo, T., Wakamatsu, T., Ishikawa, H., Nakagawa, N., Kuramitsu, S., and Masui, R.: "Insights into different dependence of dNTP triphosphohydrolase on metal ion species from intracellular ion concentrations in *Thermus thermophilus*", Extremophiles, **12**, 217-223 (2008)

(2) Iino, H., Naitow, H., Nakamura, Y., Nakagawa, N., Agari, Y., Kanagawa, M., Ebihara, A., Shinkai, A., Sugahara, M., Miyano, M., Kamiya, N., Yokoyama, S., Hirotsu, K., and Kuramitsu, S.: "Crystallization screening test for the whole-cell project on *Thermus thermophilus* HB8", Acta Cryst. **F64**, 487-491 (2008)

(3) Morita, R., Ishikawa, H., Nakagawa, N., Kuramitsu, S., and Masui, R.: "Crystal structure of a putative DNA methylase TTHA0409 from *Thermus thermophilus* HB8", Proteins **73**, 259-264 (2008)

(4) Fukui, K., Nishida, M., Nakagawa, N., Masui, R., and Kuramitsu, S.: "Bound nucleotide controls the endonuclease activity of mismatch repair enzyme MutL", J. Biol. Chem. **283**, 12136-12145 (2008)

(5) Kondo, N., Ebihara, A., Ru, H., Kuramitsu, S., Iwamoto, A., Rao, Z., and Matsuda, Z.: "*Thermus thermophilus*-derived protein tags that aid in preparation of insoluble viral proteins", Anal. Biochem. **385**, 278-285 (2009)

(6) Nakane, S., Nakagawa, N., Kuramitsu, S., and Masui, R.: "Characterization of DNA polymerase X from *Thermus thermophilus* HB8 reveals the POLXc and PHP domains are both required for 3'-5' exonuclease activity", Nucleic Acids Res. **37**, 2037-2052 (2009)

(7) Ooga, T., Ohashi, Y., Kuramitsu, S., Koyama, Y., Tomita, M., Soga, T., and Masui, R.: "Degradation of ppGpp by Nudix pyrophosphatase modulates the transition of growth phase in the bacterium *Thermus thermophilus*", J. Biol. Chem. **284**, 15449-15456 (2009)

(8) Kitamura, Y., Ebihara, A., Agari, Y., Shinakai, A., Hirotsu, K., and Kuramitsu, S.: "Structure of D-alanine-D-alanine ligase from *Thermus thermophilus* HB8: cumulative conformational change and enzyme-ligand interactions", *Acta Cryst.* **D65**, 1098-1106 (2009)

(9) Wakamatsu, T., Kitamura, Y., Kotera, Y., Nakagawa, N., Kuramitsu, S., and Masui, R.:

"Structure of RecJ exonuclease defines its specificity for single-stranded DNA", *J. Biol. Chem.* **285**, 9762-9769 (2010)
(10) Jeyakanthan, J., Drevland, R. M., Gayathri, D. R., Velmurugan, D., Shinkai, A., Kuramitsu, S., Yokoyama, S., and Graham, D. E.: "Substrate specificity deteminats of the methanogen homoaconitase enzyme: structure and function of the small subunit", *Biochemistry* **49**, 2687-2696 (2010)
(11) Wakamatsu, T., Kim, K., Uemura, Y., Nakagawa, N., Kuramitsu, S., and Masui, R.: "Role of RecJ-like protein with 5'-3' exonuclease activity in oligo(deoxy) nucleotide degradation", J. Biol. Chem. **286**, 2807-2816 (2011)

b. Oral Presentations

(1) Kuramitsu, S.: "Structural and Functional Genomics on the Extremely Thermophilic Model Organism, *Thermus thermophilus* HB8", 2008 Taiwan-Japan Proteomics Symposium, International Conference Hall, Humanities and Social Sciences, Academia Sinica, Taipei, Taiwan, Dec. (2008)
(2) Ebihara A., Shinkai A., Kanagawa M., Agari Y., Iino H., Kitamura Y., Sakamoto K., Manzoku M., Fukui K., Nakagawa N., Masui R., Bessho Y., Terada T., Shirouzu M., Yokoyama S., and Kuramitsu S. : "Structural and functional whole-cell project for the model organism, Thermus thermophilus HB8", 21th Congress and General Assembly of the International Union of Crystallography (IUCr2008), Osaka, Japan, Aug. (2008)
(3) Wakamatsu, T., Kotera, Y., Nakagawa, N., Kuramitsu, S., and Masui, R.: "Structure of RecJ exonuclease defines its specificity for single-stranded DNA", 7th 3R (Replication, Recombination and Repair) Symposium, Toyama, Japan, Oct. (2010)
(4) Shimada, A., Fukui, K., Kuramitsu, S., and Masui, R.: "Functional analysis of a novel single-stranded DNA-specific 3'-5' exonuclease involved in DNA mismatch repair", 7th 3R (Replication, Recombination and Repair) Symposium, Toyama, Japan, Oct. (2010)
(5) Bessho Y., Shinkai A., and Kuramitsu S.: "The system-biological whole-cell project of a model organism, Thermus thermophilus HB8", 8th International Congress on Extremophiles (Extremophiles 2010), Azores, Portugal, Sep. (2010)

G. Future Plans

1. Construction of Resources

Among the 2,236 total proteins, about 10% (200 proteins) of the plasmids for protein overexpression and 55% (1,200 proteins) of the plasmids for gene disruption remain to be constructed. We will construct these plasmids, because they are essential for the discovery of uncharacterized protein functions.

2. Cellular Imaging

Many particles were observed by cryo-electron tomography. In order to identify each molecule, a metal-containing tag protein will be systematically introduced to the C-terminus of the target molecule, and the position of that molecule will be observed.

3. Molecular Imaging

DNA-repair proteins are useful for fixing target proteins on DNA. The newly constructed protein with this DNA-binding domain on the N-terminal side will be used for fixing the target protein in vacuo. We will develop this protein fixation system in collaboration with Professor T. Yanagida, for single-molecule imaging for future XFEL.

H. Curriculum Vitae (Team Leader)

NAME: Seiki KURAMITSU

DATE OF BIRTH: September 9, 1949

EDUCATION:
1969-1972: Department of Biology, Faculty of Science, Osaka University
1973-1977: Graduate School of Science, Osaka University

DEGREES: Dr. Sci.

APPOINTMENTS:
1982-1986: Assistant Professor, Department of Biochemistry, Osaka Medical College
1986-1991: Associate Professor, Department of Biochemistry, Osaka Medical College
1991-: Professor, Department of Biological Sciences, Faculty of Science, Osaka University
1999-2005: Group Director, Structurome Research Group, RIKEN Harima Institute at SPring-8
2006-: Group Director, SR System Biology Research Group, RIKEN Harima Institute at SPring-8

ACADEMIC ACTIVITIES:

Protein Society
International Structural Genomics Organization (ISGO)
(2002 – 2006: Executive Committee)
The Japanese Biochemical Society
(1994 – 1996, and 1999 – 2001: Councilor,
2007 – 2009: Editor of *Journal of Biochemistry*,
2008 – 2010: Branch Manager of the Kinki Branch
2000, 2000, 2002, 2005, 2009, and 2009: JB Best Paper Award)
The Protein Science Society of Japan
(1996 – 2000, 2000 – 2007, and 2009 –: Councilor)
The Vitamin Society of Japan
(1991: Research Award)
National Committee for Biochemistry, Science Council of Japan
(2000 – 2003: Committee)
The Molecular Biology Society of Japan
The Japanese Society for Extremophiles
Society of Genome Microbiology, Japan
The Crystallographic Society of Japan
The Japanese Society for Synchrotron Radiation Research
The Chemical Society of Japan
The Biophysical Society of Japan

2-7-2. Functomics Biology I Research Team / 機能解析第１研究チーム

Team Leader; Akeo SHINKAI, Dr. Agr. / 新海　暁男
Since April 2006

A. Research Topics (Highlights)

The ultimate goal of our research group is to understand all of the fundamental biological phenomena at an atomic-resolution and to image and simulate cellular systems, using the *T. thermophilus* HB8 strain as a model organism. To achieve this goal, we have to identify or classify the functions of the remaining ~500 functionally unknown proteins in this strain.

We have been classifying the proteins by characterizing their transcriptional regulation. The bacterial RNA polymerase core enzyme binds σ factor to recognize the promoter on DNA, thus initiating transcription. In many cases, DNA-binding proteins called transcription factors regulate the transcription reaction to adapt and/or to respond to environmental alterations and stresses. Transcriptional regulation of *T. thermophilus* HB8 may be relatively simple, because this strain has been predicted to have a small number of transcriptional regulators, as compared to other microorganisms. Elucidation of the functions of transcriptional regulators will lead not only to an understanding of the essential and fundamental cell systems but also to the functional classification of the functionally unknown proteins in the strain, because the transcription of genes sharing similar cellular functions is often synchronously regulated. We will use the SPring-8 and XFEL beamlines and electron microscopy, for the molecular imaging of transcription factors and functionally unknown proteins including large protein complexes.

1. Molecular Imaging of Transcription Factors Toward Cellular Imaging.
(1) Global Transcriptional Regulators: The CRP/FNR Family Proteins

Firstly, we have focused on the global transcription factor family proteins that regulate the expression of multiple genes. We found that one of the four CRP/FNR family proteins from *T. thermophilus*, CRP, positively regulated 22 genes that may be involved in DNA/RNA metabolism, including clustered regularly interspaced short palindromic repeat (CRISPR)-associated (Cas) proteins. These proteins are thought to be involved in host defense against invading foreign replicons, such as viruses (see below). We observed that the transcription of the CRP-regulated genes increased upon phage infection in a CRP-dependent manner. Another CRP/FNR family protein, SdrP, was highly expressed in the stationary growth phase or under oxidative stress, and it positively regulated the transcription of 22 genes that may function mainly in the oxidative stress response. The crystal structure of apo-SdrP resembled that of the DNA-bound form of the *E. coli* CRP-cAMP complex, indicating that SdrP binds DNA without an effector molecule.

(2) Global Transcriptional Regulators: The TetR Family Proteins

We found that one of the four TetR family proteins, FadR, negatively regulated 21 genes that may be involved in fatty acid degradation. In the presence of a medium or long fatty acid-CoA, the FadR protein lost the ability to function as a transcriptional repressor. An X-ray crystal structure analysis revealed that FadR bound a medium chain fatty acid-CoA. The acyl chain moiety was in the center of the FadR molecule, enclosed within a tunnel-like substrate-binding pocket surrounded by hydrophobic residues, and the CoA moiety interacted with basic residues on the protein surface. We found that another TetR family protein,

TTHA0973, negatively regulated the expression of 11 genes involved in phenylacetic acid metabolism. In the presence of phenylacetyl-CoA, the TTHA0973 protein lost the ability to function as a transcriptional repressor. The three-dimensional structure of TTHA0973 was predicted by homology modeling. The putative structure adopts the typical three-dimensional structure of the TetR family proteins, with ten α-helices. A positively-charged surface, found at the center of the molecule, is similar to the acyl-CoA binding site of the *T. thermophilus* FadR molecule. The CoA moiety of phenylacetyl-CoA may bind to the center of the molecule in a similar manner to that of FadR with the CoA moiety of acyl-CoA.

(3) Copper-Sensing Transcriptional Regulator Protein CsoR

The X-ray crystal structure analysis of *T. thermophilus* CsoR indicated that the protein formed a homotetramer. In the absence of copper ions, *T. thermophilus* CsoR bound to the promoter region of the copper-sensitive operon *copZ-csoR-copA*, which encodes the copper chaperone CopZ, CsoR, and copper efflux P-type ATPase CopA, to repress their expression. In the presence of an approximatory equal amount of copper ion, CsoR was released from the DNA, to allow expression of the downstream genes. Both Cu(II) and Cu(I) ions could bind CsoR, and were effective for transcriptional de-repression. In addition, CsoR could sense various metal ions, such as Zn(II), Ag(I), Cd(II), and Ni(II), which led to transcriptional de-repression. The copper-binding motif of *T. thermophilus* CsoR comprises C-H-H, while those of most orthologs comprise C-H-C. Analyses of the X-ray crystal structure of *T. thermophilus* CsoR suggested that a histidine residue in the N-terminal domain is also involved in metal-ion binding; that is, the binding motif could be H-C-H-H, like that of *E. coli* RcnR, which binds Ni(II)/Co(II). The non-conserved H70 residue in the metal-binding motif of *T. thermophilus* CsoR is important for its DNA-binding affinity and metal-ion responsiveness.

(4) σ^E–anti-σ^E Factor Proteins

T. thermophilus HB8 has two σ factor proteins, the housekeeping σ, σ^A, which transcribes most genes, and the alternative σ, σ^E. We identified three promoters (regulating five genes) for σ^E. We found that the TTHB212 gene (*asiE*), one of the σ^E-regulated genes located downstream of the *sigE* gene in the same operon, encodes anti-σ^E factor, which binds σ^E and prevents it from binding to the RNA polymerase core enzyme. The other three σ^E-regulated genes encode functionally uncharacterized proteins.

In summary, we have elucidated the functions of seven transcriptional regulators, and categorized 84 genes, including 28 functionally unknown genes based on their transcriptional regulation.

2. Molecular Imaging of Functionally Unknown Proteins Toward Cellular Imaging.

(1) The CRISPR-Associated (Cas) Proteins

CRISPR/*cas* system is a novel prokaryotic host defense system, which was recently discovered and vigorously studied over the last several years. CRISPR is composed of direct DNA repeats composed of 24–47 bp, separated by non-repetitive, unique spacer sequences with a similar length. Sequences derived from foreign replicons, such as phages and plasmids, are found in the spacers of several CRISPRs. CRISPR loci are transcribed and processed into small CRISPR RNAs. CRISPRs are flanked by the *cas* genes, most of which encode uncharacterized proteins. The Cas proteins, together with the CRISPR RNAs, cleave foreign replicons, such as viruses. Thus, the CRISPR/*cas* system may be a prototype of the eukaryotic RNAi system. It was recently observed that the Cas proteins formed multiple complexes comprising heteromeric subunits. *T. thermophilus* HB8 is also a suitable model organism for

studying the CRISPR/*cas* host defense system because this strain has 12 CRISPR loci and 29 Cas proteins, as compared to the smaller numbers of CRISPR loci and Cas proteins in other bacteria. We determined the crystal structure of the Cse2 subunit of the Cse1–4 and Cas5e complex, which is involved in producing CRISPR RNA, and found that it adopted a novel fold comprising nine α-helices. We also determined the crystal structure of the Cmr5 subunit of the Cmr1–6 (RAMP) complex, which cleaves the invading replicon, and found that it formed a novel trimer. Both Cse2 and Cmr5 have basic patches on one side of the surface, which might interact with DNA or RNA. Recently, we successfully purified the RAMP complex from the *T. thermophilus* HB8 strain, to determine the X-ray, electron microscopy, and/or solution structures.

(2) TTHB210 Protein

We have determined the X-ray crystal structure of a functionally unknown *T. thermophilus* HB8 protein, TTHB210, which is regulated by RNA polymerase σ^E factor (see above). We found that TTHB210 adopts a novel fold with a decamer. Based on this structure, we will predict and determine the function of this protein, which will lead to the prediction of the physiological function of σ^E factor.

B. Research Subjects

(1) Molecular imaging of transcription factors and functionally unknown proteins
(2) Basic studies for molecular and cellular imaging

C. Projects

Project name	Category	Started	Completed
Functional analysis of metal-transporter like proteins from *T. thermophilus* HB8 by using X-ray fluorescence microscopy	Institute program	FY2009	FY2009
Classification of functionally unknown genes based on mRNA expression analysis	MEXT, Grant-in-Aid for Science Research (C)	FY2010	FY2012

D. Members

as of March 1st, 2011

	number	Name
Research Scientist	1	Akeo Shinkai
Technical Scientist	0	
Research Staff	2	Yoshihiro Agari, Keiko Sakamoto
Technical Staff	0	
Visiting Researchers	2	
Trainees	0	

E. Funding

(million yen)

	FY2008	FY2009	FY2010
Laboratory budget from RIKEN	3	2	2
Competitive fund in RIKEN	0	4	0
Competitive fund outside RIKEN	0	0	1
Other fund from University, Private foundations etc.	0	0	0

F. Research Output

	FY2008	FY2009	FY2010
International Publications	9	15	6
Publications in Japanese	0	0	0
Oral Presentations	11	12	12
Patent Applications	0	0	0

a. Papers

(1) Sakamoto K., Agari Y., Yokoyama S., Kuramitsu S., and Shinkai A. : "Functional identification of an anti-σ^E factor from *Thermus thermophilus* HB8", Gene 423, 153–159 (2008)
(2) Agari Y., Kashihara A., Yokoyama S., Kuramitsu S., and Shinkai A. : "Global gene expression mediated by *Thermus thermophilus* SdrP, a CRP/FNR family transcriptional regulator", Mol. Microbiol. 70, 60–75 (2008)
(3) Agari Y., Yokoyama S., Kuramitsu S., and Shinkai A. : "X-ray crystal structure of a CRISPR-associated protein, Cse2, from *Thermus thermophilus* HB8", Proteins 73, 1063–1067 (2008)
(4) Sakamoto K., Agari Y., Agari K., Yokoyama S., Kuramitsu S., and Shinkai A. : "X-ray crystal structure of a CRISPR-associated RAMP superfamily protein, Cmr5, from *Thermus thermophilus* HB8", Proteins 75, 528–532 (2009). Erratum in: Proteins 78, 1161.
(5) Agari Y., Sakamoto K., Tamakoshi M., Oshima T., Kuramitsu S., and Shinkai A. : "Transcription profile of *Thermus thermophilus* CRISPR systems after phage infection", J. Mol. Biol. 395, 270–281 (2010)
(6) Sakamoto K., Agari Y., Agari K., Kuramitsu S., and Shinkai A. : "Structural and functional characterization of transcriptional repressor CsoR from *Thermus thermophilus* HB8", Microbiology 156, 1993–2005 (2010)
(7) Agari Y., Kuramitsu S., and Shinkai A. : "Identification of novel genes regulated by the oxidative stress-responsive transcriptional activator SdrP in *Thermus thermophilus* HB8", FEMS Microbiol. Lett. 313, 127–134 (2010)
(8) Agari Y., Agari K., Sakamoto K., Kuramitsu S., and Shinkai A. : "TetR family transcriptional repressor *Thermus thermophilus* FadR controls fatty acid degradation", Microbiology, in press. (doi: 10.1099/mic.0.048017-0)

b. Oral Presentations (* Invited presentation)

(1) Agari Y., Sato S., Wakamatsu T., Bessho Y., Ebihara A., Yokoyama S., Kuramitsu S., Shinkai A. : "X-ray crystal structure of a hypothetical Sua5 protein from *Sulfolobus*

tokodaii strain 7", 21th Congress and General Assembly of the International Union of Crystallography (IUCr2008), Osaka, Japan, Aug. (2008)

(2) Sakamoto K., Agari Y., Yokoyama S., Kuramitsu S., and Shinkai A. : "Functional identification of protein from *Thermus thermophilus* HB8: Identification of an anti-σ^E factor", 31th Annual Meeting of the Molecular Biology Society of Japan/ 81th Annual Meeting of the Japanese Biochemical Society (BMB2008), Kobe, Japan, Dec. (2008)

(3) Shinkai A., Agari Y., and Sakamoto K. : "Transcriptional regulation of *Thermus thermophilus* HB8: Functional identification of transcription factors and classification of functionally uncharacterized genes", Symposium on the 82nd Annual Meeting of the Japanese Biochemical Society, Kobe, Japan, Oct. (2009)*

(4) Shinkai A. : "Study of CRISPR anti-virus system using *Thermus thermophilus* HB8 as a model organism", Workshop on the 32th Annual Meeting of the Molecular Biology Society of Japan, Yokohama, Japan, Dec. (2009)*

(5) Shinkai A. : "Functional and structural genomics studies on *Thermus thermophilus* CRISPR/*cas* systems", Meeting on CRISPR Mechanisms & Applications, Wageningen, Netherlands, Oct. (2010)*

(6) Sakamoto K., Agari Y., Agari K., Kuramitsu S., and Shinkai A. : " Structure and function of transcriptional repressor CsoR from *Thermus thermophilus* HB8", 33th Annual Meeting of the Molecular Biology Society of Japan/ 83th Annual Meeting of the Japanese Biochemical Society (BMB2010), Kobe, Japan, Dec. (2010)

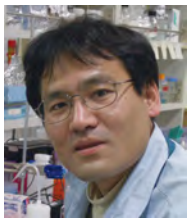
(7) Agari Y., Kuramitsu S., and Shinkai A. : "Oxidative stress responsive transcriptional regulation mediated by SdrP in *Thermus thermophilus* HB8", 33th Annual Meeting of the Molecular Biology Society of Japan/ 83th Annual Meeting of the Japanese Biochemical Society (BMB2010), Kobe, Japan, Dec. (2010)

(8) Agari Y., Agari K., Sakamoto K., Kuramitsu S., and Shinkai A. : "Structure and function of TetR family transcriptional repressor *Thermus thermophilus* FadR which controls fatty acid degradation", 33th Annual Meeting of the Molecular Biology Society of Japan/ 83th Annual Meeting of the Japanese Biochemical Society (BMB2010), Kobe, Japan, Dec. (2010)

G. Future Plans

The ultimate goal of our research group is to understand all fundamental biological phenomena at an atomic-resolution (in terms of physical chemistry) and to image and simulate cellular systems, using the *T. thermophilus* HB8 strain as a model organism. To achieve this goal, we will classify the remaining ~500 functionally unknown proteins by characterizing their transcriptional regulation. In order to do this, we will functionally identify the remaining transcription factors, especially focusing on the global transcriptional regulator family proteins that regulate the expression of multiple genes, by both biochemical and structural studies. We will also focus on the CRISPR/*cas* defense system, which was recently discovered and extensively studied over the last several years. *T. thermophilus* HB8 is suitable for studying this system because it has multiple CRISPR/*cas* genes, i.e., 12 CRISPR loci and 29 Cas proteins, as compared to other bacteria; furthermore, thermostability of the proteins from this strain facilitates structural and functional analyses. Since the high resolution structures of the large Cas protein complexes are one of the top concerns in this field, we will prepare them from this strain, and determine their crystal, electron microscopy, and/or solution structures, using the SPring-8 and XFEL beamlines, in collaboration with laboratories at the SPring-8 center. In the long-term future, we will develop strategies to image the host defense system functioning *in vivo*.

H. Curriculum Vitae (Team Leader)



NAME: Akeo SHINKAI

DATE OF BIRTH: May 8, 1963

EDUCATION:
1986: Graduated from school of Agriculture, Nagoya University
1988: Master Degree from Graduate school of Agriculture, Nagoya University
1991: Dr. Agriculture from Graduate school of Agriculture, The University of Tokyo

ACADEMIC DEGREES: Dr. Agr.

APPOINTMENTS:
1991-2002 : Research Scientist, Tokyo Research Laboratories, Kyowa Hakko Kogyo, Co., Ltd.
1999-2001 : Visiting Scientist (concurrent), Department of Pathology, University of Washington
2002-2006 : Senior Research Scientist, RIKEN SPring-8 Center, Harima Institute
2006-present : Present post
2009-present : Invited Researcher (concurrent), Graduate School of Science, Osaka University
2011 : Visiting Lecturer (concurrent), Graduate School of Science, Osaka University

ACADEMIC ACTIVITIES:
The Molecular Biology Society of Japan
The Protein Science Society of Japan
The Japanese Biochemical Society

2-7-3. Functomics Biology II Research Team / 機能解析第２研究チーム

Team leader; Yoshitaka BESSHO, Ph. D. / 別所 義隆
Since Apr 2006,

A. Research Topics (Highlights)

The mission of the team is to accomplish the complete elucidation of intracellular molecular systems, through structural and functional analyses. We are focusing on the "protein-synthesis (translation)" and "DNA-repair" systems, as essential cellular processes in the central-dogma of life. The protein synthesis system is the most important part of the cell operations. Translation is a compiling system, from the genetic information of the DNA to the amino acid chain of the protein. The translator molecule is “tRNA”, the place of translation is the “ribosome”, and the rule of translation is “the genetic code”. tRNA is a key molecule of the protein synthesis system, and thus we have focused on the enzymes related to tRNA maturation and aminoacylation.

1. Structural and functional analyses of the protein-synthesis systems of life.

tRNAs are ribonucleic acids, and are first synthesized as non-functional transcripts. As a consequence of “Splicing”, “Excision”, “Terminal trimming” and “Mending”, the tRNAs are matured into functional molecules. Posttranscriptional modifications are important for helping the tRNA to fold correctly, in each processing step. A single tRNA molecule has 9 modified nucleotides, on average. Simple methylation, isomerization and deamination are primitive modifications in the evolution of life. In addition, thiolation, reduction, and alkylation are often observed. Amino acids and metals are occasionally used as co-factors. There are more than 40 kinds of tRNA in an organism. For each tRNA to function correctly in translation, chemical modifications are required. At least 100 kinds of modified bases have been reported, thus far.

Bio-molecular imaging of multiple tRNA complexes involved in the maturation system

Since approximately 15 modification enzymes are involved in the maturation of each tRNA, the question arises as to how tRNAs are modified at the multiple nucleotides and by the corresponding enzymes during their processing. We focused on the “cooperation” of the modification molecules for understanding the processing system, i.e., the 3D interactome of proteins and substrates. During the maturation steps, the tRNA should be modified to fold in the correct chronological order. We adopted a model in which the earlier-functioning modification enzymes bring the enzymes needed for the next step, as in a cascade reaction, one after another. This is the hypothesis of the modificasome. It is like a snapshot, but not of a single molecule. We have checked for the direct associations between the enzymes in the absence of tRNA substrates.

tRNA modification enzymes, essential for the genetic-code system of the central dogma

Some tRNA modification enzymes are essential for the genetic-code system of the central dogma. Posttranscriptional modification of the wobble uridine at position 34 of the anticodon allows accurate and efficient decoding of the genetic code. In particular, the decoding of the synonymous two-codon set specific for Leu, Gln, Lys, Glu and Arg in Bacteria mainly depends on the presence of the methylene carbon on the C5 atom of U34 (xm^5U), combined with the thiolation of C2 (xm^5s^2U) or the methylation of the 2'-hydroxyl of ribose-34 (xm^5Um). Together with the type of purine nucleotide modification at position 37, adjacent to the anticodon xm^5UNN, such xm^5U34-containing tRNAs are able to decode efficiently and accurately only the pyrimidine-ending codons in the correct reading frame (no frameshift). The various enzymes involved in the formation of these essential xm^5U34 derivatives have

been identified. To clarify in structural terms how some of these enzymes (mainly GidA and MnmE) work together to catalyze the formation of the wobble xm^5U derivative, we have determined the crystal structures of the enzymes and revealed their relationships with other modification enzymes that also act on carbon-5 of uridines at other positions in tRNA.

2. Characterization and structural analyses of the DNA-repair system enzymes.

In cells, a vast amount of DNA damage occurs from UV radiation, various chemical reagents, and errors during DNA replication and genetic recombination. This damage is very harmful, and can result in mutagenesis and even cell death. To remove these lesions, cells have various types of DNA repair systems, and most of them are common to many organisms, ranging from bacteria to human.

Structural analyses of DNA repair enzymes

In this project, we determined the crystal structures of DNA repair enzymes from *T. thermophilus*. The structure of RecJ, a single-stranded DNA-specific 5'-3' exonuclease required for various DNA repair pathways, clearly revealed that the characteristic ring-like structure is a key feature to achieve its specificity for single-stranded DNA. We also determined the crystal structure of *T. thermophilus* uracil DNA glycosylase (UDG) complexed with a substrate DNA. The UDG enzyme removes the uracil generated by the deamination of cytosine or the misincorporation of deoxyuridine monophosphate. This structure suggested not only the catalytic mechanism of the enzyme but also the universal damage-recognition mechanism conserved among all UDG superfamily members.

Characterization of novel genome-maintenance mechanisms

In *E. coli*, O^6-methylguanine DNA methyltransferase (Ogt) transfers the methyl group from a damaged base to a cysteinyl residue in the enzyme. We have found that *T. thermophilus* Ogt interacts with UvrA, a nucleotide excision DNA repair enzyme, suggesting that *T. thermophilus* Ogt acts as a sensor protein to recruit the nucleotide excision repair enzymes to the lesion.

In vitro reconstitution of the DNA mismatch repair system and biological applications

Since the protein-protein interactions in the subsystems profoundly impact the activity of each enzyme, system biological analyses must reconstitute the DNA repair subsystems *in vitro* and characterize each reaction step in the presence of the interacting partners. We attempted the *in vitro* reconstitution of the DNA mismatch repair subsystem, which corrects mismatched base pairs mainly caused by replication errors. A plasmid DNA containing a mismatch at a restriction site was constructed, and we assessed the repair activity by monitoring the recovery of the sensitivity to restriction enzyme digestion. Our *in vitro* reconstituted DNA mismatch repair system consists of 8 proteins and repaired the mismatched plasmid DNA to some extent.

3. Origin and evolution of fundamental molecular systems essential for the living cell.

The cell, the fundamental unit of life, is a molecular system consisting of a variety of chemical compounds, such as proteins, nucleic acids, lipid bilayers and polysaccharides. In contemporary organisms, these compounds are respectively synthesized from amino acids, nucleotides, lipids and sugars, as the basic units. Since the organic compounds produced prebiotically were exhausted in the early days of life, the organisms had to develop machinery to synthesize such compounds for sustaining life. This self-organization system must be traceable within the genomes of contemporary organisms. In this project, we searched for the trace of this integration in the genome. Our recent progress in structural biology, biochemistry, and molecular biology has encouraged us in our challenge to elucidate the origin and evolution of the fundamental molecular systems essential for the living cell.

4. Development of a bio-molecular imaging method toward frontier coherent X-ray FEL.

Coherent imaging is a growing field in optical science. We are developing methods to visualize protein and nucleic-acid complexes and their interactions at higher resolution, by

combinations of various technologies, as described below.

Solution scattering of RNA and protein complexes by using a nano bio-device

We are developing cutting-edge technologies of bio-molecular imaging, facilitated by new generation pulsed coherent X-rays. Molecular interactions and dynamic reactions will be measured with high quality under almost natural cellular conditions, revealing the complicated molecular mechanisms in living systems. For this purpose, we have successfully elucidated the solution structure of a protein and RNA complex by conventional small angle X-ray scattering. In addition, we performed effective computer simulations using coarse graining models, and designed a nano bio-device toward the biological application of XFEL/SPring-8.

Tag system of DNA-repair proteins toward single molecular imaging

Fluorescently-tagged protein domains are useful for *in vitro* imaging of the target molecules. As single-molecule imaging analyses, we will attempt to visualize protein-DNA interactions at high resolution. We have started with DNA repair systems as a model, because about 10 proteins involved in this system, which show very high affinity to damaged DNA, have been obtained. Since the proteins from *T. thermophilus* are stable in a vacuum, we will develop a technology to place a protein molecule onto a DNA molecule. This technology will contribute to single-molecule imaging in the future with XFEL.

B. Research Subjects

(1) System biological research of enzymes in the central dogma system of life.
(2) Elucidation of the origin and evolution of fundamental molecular systems.
(3) Research and Development of bio-molecular imaging method for XFEL.

C. Projects

Project name	Category	Started	Completed
Structural and functional analysis of homologous recombination-suppressing system.	MEXT, Grants-in-Aid for Young Scientists (Start-up)	2009	2009
Application of effective post-labeling method using by RNA methyltransferases and synthetic AdoMet-derivatives.	MEXT, Grants-in-Aid for Scientific Research (C)	2009	2011
Research and development of bio-molecular imaging method using a frontier coherent X-ray diffraction.	MEXT/ JST/ Cooperative Research Program (Network Joint Research Center for Materials and Devices)	2010	2010

D. Members

as of March 1st, 2011

	number	Name
Research Scientist	3	Yoshitaka Bessho, Kenji Fukui, Aya Kitamura
Technical Scientist	0	
Research Staff	1	Hitoshi Iino
Technical Staff	0	

Visiting Researchers	11	
Trainees	0	

E. Funding

(million yen)

	FY2008	FY2009	FY2010
Laboratory budget from RIKEN	3	2	2
Competitive fund in RIKEN	0	3	0
Competitive fund outside RIKEN	0	2	1
Other fund from University, Private foundations etc.	0	0	0

F. Research Output

	FY2008	FY2009	FY2010
International Publications	8	17	6
Publications in Japanese	0	0	0
Oral Presentations	24	17	26
Patent Applications	0	0	0

a. Papers (from last RSAC)

(1) Agari Y., Sato S., Wakamatsu T., Bessho Y., Ebihara A., Yokoyama S., Kuramitsu S., and Shinkai A. : "X-ray crystal structure of a hypothetical Sua5 protein from *Sulfolobus tokodaii* strain 7", Proteins. 70(3), 1108-1111 (2008)

(2) Ihsanawati, Nishimoto M., Higashijima K., Shirouzu M., Grosjean H., Bessho Y., and Yokoyama S. : "Crystal structure of tRNA *N2,N2*-guanosine dimethyltransferase Trm1 from *Pyrococcus horikoshii*", J Mol Biol. 383(4), 871-884 (2008)

(3) Ohama T., Inagaki Y., Bessho Y., and Osawa S. : "Evolving genetic code.", Proc Jpn Acad Ser B Phys Biol Sci. 84(2), 58-74 (2008)

(4) Awai T., Kimura S., Tomikawa C., Ochi A., Ihsanawati, Bessho Y., Yokoyama S., Ohno S., Nishikawa K., Yokogawa T., Suzuki T., and Hori H. : "*Aquifex aeolicus* tRNA (*N2,N2*-guanine)-dimethyltransferase (Trm1) catalyzes transfer of methyl groups not only to guanine 26 but also to guanine 27 in tRNA", J Biol Chem. 284(31), 20467-20478 (2009)

(5) Bessho Y. and Yokoyama S. : "Enzymatic formation of 5-aminomethyl-uridine derivatives in tRNA", In: Henri Grosjean (ed) DNA and RNA modification enzymes. Landes Bioscience, Austin, pp.409-425 (2009)

(6) Kuratani M., Hirano M., Goto-Ito S., Itoh Y., Hikida Y., Nishimoto M., Sekine S., Bessho Y., Ito T., Grosjean H., Yokoyama S. : "Crystal structure of *Methanocaldococcus jannaschii* Trm4 complexed with sinefungin", J Mol Biol. 401(3), 323-333 (2010)

(7) Hikida Y., Kuratani M., Bessho Y., Sekine S.I., and Yokoyama S. : "Structure of an archaeal homologue of the bacterial Fmu/RsmB/RrmB rRNA cytosine 5-methyltransferase", Acta Crystallogr D Biol Crystallogr. 66(Pt12), 1301-1307 (2010)

(8) Kuratani M., Kasai T., Akasaka R., Higashijima K., Terada T., Kigawa T., Shinkai A., Bessho Y., and Yokoyama S. : "Crystal structure of *Sulfolobus tokodaii* Sua5 complexed with L-threonine and AMPPNP", Proteins. DOI:10.1002/prot.23026 (2011)

b. Oral Presentations (* Invited presentation)

(1) Ebihara A., Shinkai A., Kanagawa M., Agari Y., Iino H., Kitamura Y., Sakamoto K., Manzoku M., Fukui K., Nakagawa N., Masui R., Bessho Y., Terada T., Shirouzu M.,

Yokoyama S., and Kuramitsu S. : "Structural and functional whole-cell project for the model organism, *Thermus thermophilus* HB8", 21th Congress and General Assembly of the International Union of Crystallography (IUCr2008), Osaka, Japan, Aug. (2008)

(2) Ito Y., Chiba S., Naganuma M., Ito S., Fukunaga R., Kuratani M., Bessho Y., Ito T., Sekine S., and Yokoyama S. : "Crystallographic Studies of Aminoacyl-tRNA Synthesis and tRNA Modification", 23rd tRNA Workshop: from the origin of life to biomedicine, Aveiro, Portugal, Jan. (2010)

(3) Ito T., Ito S., Kuratani M., Bessho Y., and Yokoyama S. : "Tertiary structure checkpoint in tRNA functional maturation", 23rd tRNA Workshop: from the origin of life to biomedicine, Aveiro, Portugal, Jan. (2010)

(4) Bessho Y., Shinkai A., and Kuramitsu S. : "The system-biological whole-cell project of a model organism, *Thermus thermophilus* HB8", 8th International Congress on Extremophiles (Extremophiles 2010), Azores, Portugal, Sep. (2010)*

(5) Bessho Y. : "Development of RNA/RNP bio-molecular imaging method by SPring-8 coherent X-rays (XFEL)", 3rd Astrobiology workshop, Tokyo, Japan, Oct (2010)*

(6) Bessho Y. : "Chemical modification of nucleic acids and their indispensable materials", BMB2010 workshop 2W21: Origin and evolution of primary biomaterials for common cellular activities, Kobe, Japan, Dec. (2010)*

(7) Nishino Y., Tanaka Y., Ito K., Takahashi Y., Mimura H., Matsuyama S., Maeshima K., Shimura M., Joti Y., Oroguchi T., Bessho Y., Takeuchi S., Okada M., Okaya M., Nozaki K., Oji Y., Matsushita Y., Tsutsumi R., Yabashi M., Nagasono M., Togashi T., Ohashi H., Matsui S., Matsubara E., Yamauchi K., and Ishikawa T. : "Coherent Imaging using Synchrotron Radiation and FEL", Biology with FELs: Toward the Molecular Moview, Berkeley, California, Jan (2011)

G. Future Plans

1. Elucidation of the draft map of the translation system.

Our aim is to establish the complete elucidation of the intracellular subsystems, through structural and functional analyses. Comparisons of the reaction rates of the systems by *in vivo* and *in vitro* analyses could provide information about unknown intracellular regulatory mechanisms. Therefore, we will establish the reconstituted tRNA-maturation subsystems *in vitro*, and carry out the kinetic analyses. We will perform comprehensive structural analyses of the multi-functional complexes in the translation systems. These analyses are expected to reveal the draft map of the molecular systems, and the methodology established in this study should be applicable to other systems involved in cellular processes. The research encourages the challenge to elucidate the origin of the fundamental molecular systems essential for the living cell.

2. Development research of bio-molecular coherent imaging, using synchrotron radiation and XFEL technology.

This team will address the development of molecule imaging technologies of solution structures, by using the SPring-8 and XFEL beamlines. Coherent imaging is a growing field in optical science. We are planning to visualize protein and nucleic-acid interactions at higher resolution. Rather than using a lens for image formation, coherent imaging instead numerically reconstructs the object images from the coherent diffraction data. In collaboration with Dr. Nishino’s group at Hokkaido University, as well as the XFEL team of RIKEN Harima Institute, we will perform computer simulations for biomolecular solution scattering, utilizing the pulse coherent X-ray of XFEL. For the measurement of bio-molecular scattering with the XFEL beam, we will develop a nano bio-device with a micro channel, in collaboration with Dr. Takeuchi of Tokyo University.

H. Curriculum Vitae (Team Leader)

NAME: Yoshitaka BESSHO

DATE OF BIRTH: February 6, 1966

EDUCATION:

1985-1988: Department of Biology, Faculty of Science, Shizuoka University

1989-1992: Graduate School of Science, Nagoya University

ACADEMIC DEGREES: Dr. Sci.

APPOINTMENTS:

1992-1999: Assistant Professor, Graduate School of Science, Nagoya University.

1998-1999: Japanese Governmental Overseas Research Fellow, in New York State University.

2000-2001: Post-doctoral Researcher, New York State University.

2001-2003: Scientist, Genomic Sciences Center, RIKEN Yokohama Institute.

2004-2007: Senior Scientist, Genomic Sciences Center, RIKEN Yokohama Institute.

2006-2009: Senior Scientist, SR System Biology Research Group, RIKEN Harima Institute at SPring-8 (Concurrent position).

2008-2009: Senior Scientist, Systems and Structural Biology Center, RIKEN Yokohama Institute.

2009-present: Team Leader, Functomics Biology II Research Team, SR System Biology Research Group, RIKEN Harima Institute at SPring-8.

ACADEMIC ACTIVITIES:

Molecular Biology Society of Japan.

Japan RNA Society.

Society of Evolutionary Studies Japan.

The Japanese Biochemical Society.

Japan Astrobiology Network.

Japanese Society for Extremophiles.

The Japanese Society for Synchrotron Radiation Research.

2-8. Quantum Order Research Group / 量子秩序研究グループ

Group Director Masaki Takata, Ph.D. / 高田　昌樹
Since April 2007

A. Outline of the Research Group

To build new bridges between Photon Science and Materials Science

In Materials Science, extremely high brilliance synchrotron radiation (SR) is widely recognized as a powerful tool for investigating the relation between material structure and material properties. The Photon Science group/team/division/facility at SPring-8 has explored various advanced materials, such as high-Tc superconductors, MOF (Metal Organic Framework) materials, hydrogen storage materials, and thermoelectrics. There continues to be strong demand for further progress in Photon Science to expand the frontiers of Materials Science.

In 2006, the RIKEN SPring-8 Center (RSC) launched a new research organization with three strategic divisions: Innovative Light Sources, Photon Science Research, and Advanced Photon Technology. Their missions are, respectively, to produce concepts leading to newer light sources, to develop science accessible with these light sources, and to generalize the new science and related technology for wide application. In particular, two PI(Principal Investigator) laboratories in the Photon Science Research division, the Takata Structural Materials Science Laboratory and the Baron Materials Dynamics Laboratory, have been carrying out a mission to build a bridge between Photon Science and Materials Science, in cooperation with other divisions. The “Quantum Order Research Group (QORG)”, was organized in 2007 to establish RIKEN’s leadership in Materials Science using SR at SPring-8. The QORG is a task force that was formed to promote novel Materials Science and explore new research fields based on the advanced Photon Science emerging from the RSC. The success of the project will pave the way to build a collaborative research network at the frontiers of Materials Science.

To Elucidate Electronic “Quantum Order” in Materials

The term “Quantum Order” refers to the microscopic organization (energy levels, charge density, spin density, etc) of electrons in materials, as related to macroscopic material properties. Because of its direct interaction with electrons, using synchrotron radiation as a probe is well suite to elucidation of quantum order. Thus, QORG was launched at SPring-8 to promote advanced materials science, leveraging the distinct characteristics (high brilliance, short-pulse, polarization, etc.) of SPring-8 X-rays. The group formed three teams to focus on each of the key ingredients of the quantum order: “Electron Spin Order”, “Electron Spatial Order” and “Excitation Energy Order”. Their common mission is to develop advanced diffraction, scattering and spectroscopic measurement methods in order to establish innovative Quantum Order Science at SPring-8.

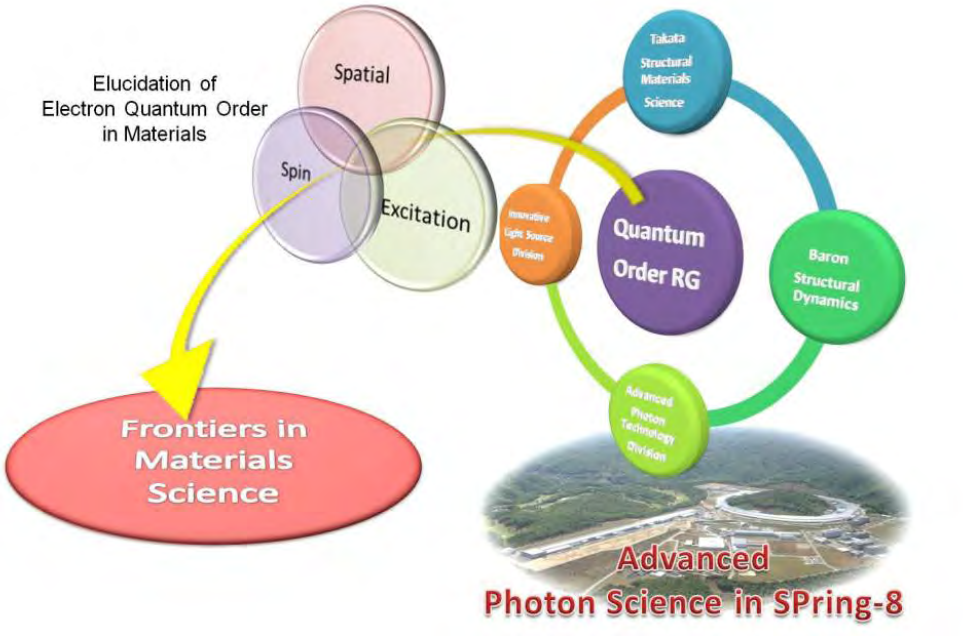
The Spin Order Research Team opens a window on advanced magnetic structural materials science by thoroughly exploiting the high performance of the SPring-8 light source. In particular, manipulation of X-ray polarization considerably improves magnetic diffraction techniques considerably.

The Spatial Order Research Team uses synchrotron radiation to advance structural materials science with synchrotron radiation. The team is upgrading charge density

distribution imaging techniques in order to find ways to design new materials from the “bottom-up”, with a focus on polymers with regular pores on nanometer length-scales.

The Excitation Order Research Team develops cutting edge spectroscopy using soft X-rays to meet the challenge of measuring electron states of hyper-complex materials like liquids and biological materials are challenging tasks.

These teams share their common mission with the RSC laboratories and are breaking ground on the frontiers in Materials Science with the innovative approaches developed at SPring-8.



Mission of the Collaborative Research Project, ‘Quantum Ordering’

B. Funding for the Research Group

(million yen)

	2006	2007	2008	2009	2010
Government Budget	—	19	19	17	16
Grants	—	0	2	2	2
Private & Others Sources	—	0	0	0	0
Spin Order Research Team	—	40	29	30	34
Spatial Order Research Team	—	30	21	23	18
Excitation Order Research Team	—	84	67	97	47

2-8-1. Spin Order Research Team / スピン秩序研究チーム

Team Leader; Taka-hisa ARIMA, Ph. D. / 有馬 孝尚
Since April 2007

A. Research Topics (Highlights)

1. Magnetic structure and wave function in a 5d transition metal oxide

In 3*d* transition-metal compounds, each magnetic moment is almost identical to $-g\mu_B S$, because of the quenching of *L* in a ligand field. In contrast, the magnetic moment at a lanthanide ion is generally determined by the total angular momentum *J*=*L*+*S*. The contracted 4*f* orbital and the large atomic number make the LS coupling much more significant than the ligand field effect. For the magnetic moment at a 5*d* transition element, the competition between the spin-orbit interaction and the ligand field effect is not as clear as in the case of 3*d* and 4*f* transition elements. We performed a study of resonant x-ray magnetic diffraction in Sr_2IrO_4. Magnetic reflections are observed at (1 0 4*n*) and (0 1 4*n*+2), where *n* is an integer. The resonant enhancement of magnetic reflections is extremely large at the L_3 edge but almost absent at the L_2 edge, implying that the orbital momentum is not quenched at each Ir^{4+} ion. Such a unique state in 5*d* transition-metal compounds would cause extraordinary electro-magnetic and magneto-optical responses. We also measured the dependence of the intensity of a magnetic reflection on the polarization of the incident beam by using a newly developed polarization rotator and estimated the L/S ratio to be around 5, which clearly proves the unquenched orbital momentum.

2. Investigation of the relationship between the sense of helimagnetism and the ferroelectric polarization direction by circularly polarized x-ray diffraction

Recent intensive studies on so-called multiferroics have revealed that the cycloidal (i.e., transverse helical) magnetic order should induce ferroelectric polarization. Such a cycloidal magnet is often modified by the application of a relatively weak magnetic field. This also accompanies the change of the ferroelectric polarization and hence shows up as a giant magnetoelectric effect. In such a spin-origin ferroelectric, the sense of the helimagnetic order should be correlated with the direction of electric polarization. According to M. Blume and D. Gibbs, the sense should be detected as a difference in intensity of x-ray magnetic reflection. We carried out circularly polarized x-ray magnetic diffraction on several typical ferroelectric helimagnets and found a difference in the intensity of a magnetic reflection in the ferroelectric phase of $MnWO_4$, $DyMnO_3$, and $(Eu,Y)MnO_3$. The spin chirality was confirmed to be switched with the reversal of electric polarization. The magnetic diffraction of a circularly polarized x-ray may be a suitable tool for investigating the change in spin chirality upon a magnetic-field-induced electric phase transition in a multiferroic, because the polarization of the x-ray beam is not modified by the application of a magnetic field.

3. Investigation of crystallographic chirality by resonant circularly-polarized x-ray diffraction

In an enantiomorphic crystal, some forbidden reflections become allowed at the absorption edge of a constituent element. The reflectivity can then be different for left- and right-handed circularly polarized x-ray beams resulting from the ordering or chirality of the material. This was found by Shin's group, who measure diffraction from quartz rcystals of out a circularly-polarized soft-x-rays. However, the long wavelength of soft x-rays means they can only diffract from a very limited number of reciprocal lattice points. We carried out a

systematic investigation of the circular-polarization dependence of the forbidden reflections in a chiral system $CsCuCl_3$ using hard x-rays. The copper chloride belongs to a $P6_122$ and $P6_522$ enantiomorphic pair, where the (0 0 *l*) reflections are allowed only when *l*=6n. At around Cu K absorption edge, (0 0 6n+2) and (0 0 6n-2) reflections are clearly observed and their intensities are dependent on the circular polarization of the incident x-ray beam. The obtained flipping ratios are quantitatively explained by taking the anisotropic x-ray susceptibility of the copper ion into account.

B. Research Subjects

(6) Investigation of magnetic structure by means of x-ray scattering
(7) Investigation of spin and orbital angular momenta at magnetic sites
(8) Investigation of crystallographic chirality by resonant x-ray scattering

C. Projects

Project name	Category	Started	Completed
Quantum Science on Strong Correlatipon	JSPS, FIRST	2010	2014

D. Members

as of March 1st, 2011

	number	Name
Research Scientist	3	Taka-hisa Arima, Hiroyuki Ohsumi, Soshi Takeshita
Technical Scientist	0	
Research Staff	0	
Technical Staff	1	Hirofumi Kodera
Visiting Researchers	3	
Trainees	7	

E. Funding

(million yen)

	FY2008	FY2009	FY2010
Laboratory budget from RIKEN	29	30	26
Competitive fund in RIKEN	0	0	0
Competitive fund outside RIKEN	0	0	8
Other fund from University, Private foundations etc.	0	0	0

F. Research Output

	FY2008	FY2009	FY2010
International Publications	9	11	3
Publications in Japanese	0	7	1
Oral Presentations	21	37	21
Patent Applications	0	0	0

a. Papers

(1) Yu X. ,Arima T. ,Seki S. ,Asaka T. ,Kimoto K. ,Tokura Y. ,and Matsui Y. : "Effect of Quenched Disorder on Charge Ordering Structure in $RE_{1.67}AE_{0.33}NiO_4$(RE=La, Pr, Nd, Sm; AE = Ca,Sr)", J. Phys. Soc. Jpn. **77**, No. 9, pp.093709-1--093709-4 (2008).

(2) Kida N. ,Ikebe Y. ,Takahashi Y. ,He J. P. ,Kaneko Y. ,Yamasaki Y. ,Shimano R. ,Arima T. ,Nagaosa N. ,and Tokura Y. : "Electrically driven spin excitation in the ferroelectric magnet $DyMnO_3$", Phys. Rev. B **78**, 104414-1--104414-9 (2008).

(3) Takahashi Y. ,Kida N. ,Yamasaki Y. ,Fujioka J. ,Arima T. ,Shimano R. ,Miyahara S. ,Mochizuki M. ,Furukawa N. ,and Tokura Y. : "Evidence for an Electric-Dipole Active Continuum Band of Spin Excitations in Multiferroic $TbMnO_3$", Phys. Rev. Lett. **101**, 187201-1--187201-4 (2008).

(4) Arima T. : "Magneto-electric optics in non-centrosymmetric ferromagnets", J. Phys.: Condens. Matter **20**, No. 43, pp.434211-1--434211-9 (2008).

(5) Taniguchi K. ,Abe N. ,Umetsu H. ,Katori H. ,and Arima T. : "Control of the magnetoelectric domain-wall stability by a magnetic field in a multiferroic $MnWO_4$", Phys. Rev. Lett. **101**, No. 20, pp.207205-1--207205-4 (2008).

(6) Nakajima T. ,Mitsuda S. ,Inami T. ,Terada N. ,Ohsumi H. ,Prokes K. ,and Podlesnyak A. : "Identification of microscopic spin-polarization coupling in the ferroelectric phase of magnetoelectric multiferroic $CuFe_{1-x}Al_xO_2$", PHYSICAL REVIEW B **78**, No. 2, pp.024106-1--024106-10 (2008).

(7) Arima T.: "Sliding electrons take charge", Nature Materials, 7(1), 12-13 (2008).

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(11) Sagayama H., Abe N., Taniguchi K., Arima T., Yamasaki Y., Okuyama D., Tokura Y., Sakai S., Morita T., Komesu T., Ohsumi H., and Takata M.: "Observation of Spin Helicity Using Non-resonant Circularly Polarized X-ray Diffraction", J. Phys. Soc. Jpn. 7, 043711-1 - 043711-4 (2010).

(12) Kuriyama H., Matsuno J., Niitaka S., Uchida M., Hashizume D., Nakao A., Sugimoto K., Ohsumi H., Takata M., and Takagi H.: "Epitaxially stabilized iridium spinel oxide without cations in the tetrahedral site", Applied Physics Letters 96, 182103-1 - 182103-3 (2010).

(13) Tokunaga Y., Kaneko Y., Okuyama D., Ishiwata S., Arima T., Wakimoto S., Kakurai K., Taguchi Y., Tokura Y.:”Multiferroic M-type hexaferrites with a room-temperature conical state and magnetically controllable spin helicity”, Phys. Rev. Lett. 105, 257201 (2010).

b. Oral Presentations (* Invited presentation)

(1) Ohsumi H.: "Advances in X-ray Magnetic Diffraction by Using Optimun Polarization", ESRF, SPring-8, APS Three-Way Meeting, Argonne, 3 月 (2008).
(2) Arima T.: "Neutron and X-ray Diffraction Studies on Spin-driven Ferroelectrics", 7th International Workshop on Polarized Neutrons in Condensed Matter Investigationc (PNCMI2008) , (Quantum Beam Science Directorate, JAEA), Tokai-mura, Ibaraki Pref. , Sept. (2008).*
(3) Okuyama D . ,Aoyagi S . ,Sugimoto K . ,Moriyoshi C . ,Ohsumi H . ,Shih C . ,Okabayashi H . ,Satou R . ,Hashimoto T . ,Nishibori E . ,Kuroiwa Y . ,Sawa H . ,Takata M . ,Tokunaga Y . ,Kaneko Y . ,Taguchi Y . ,Arima T . ,and Tokura Y . : "Accurate structure analysis of $DyMnO_3$ single crystal utilizing high flux xrays and a large cylindrical imaging plate at SPring-8", 2nd International Symposium on Anomalous Quantum Materials (ISAQM2008) and the 7th Asia-Pacific Workshop , Tokyo , Oct. (2008).
(4) Takagi H . ,Kim B . ,Fujiyama S . ,Ohsumi H . ,Arima T . ,Matsuno J . ,Hirai D . ,and Ohashi K . : "Wave function of spin-orbit complex in 5d mott insulator Sr_2IrO_4 probed by resonant magnetic X-ray diffraction", 9th Korea-Japan-Taiwan Symposium on Strongly Correlated Electron Systems , Tamshui , Taiwan , Nov. (2008).*
(5) Wakabayashi Y., Sagayama H., Arima T., Nakamura M., Ogimoto Y., Miyano K., and Sawa H.: "Effect of the substrate on the orbital phase transition in a manganite thin film under magnetic field", 2009 APS March Meeting , (American Physical Society), Pittsburgh , USA , Mar. (2009).
(6) Taguchi Y . ,Ishiwata S . ,Tokunaga Y . ,Furukawa N . ,Sakai H . ,Murakawa H . ,Onose Y . ,Arima T . ,and Tokura Y . : "Magnetically-induced electric polarization in ferrites", AIST-RIKEN Joint Workshop on ``Emergent Phenomena of Correlated Materials" , Okinawa , Mar. (2009).*
(7) Takagi H . ,Kim B . ,Fujiyama S . ,Ohsumi H . ,Arima T . ,Matsuno J . ,Hirai D . ,and Ohashi K . : "Novel Quantum Phases in 5d Ir Oxides Induced by Strong Spin-Orbit Coupling", AIST-RIKEN Joint Workshop on ``Emergent Phenomena of Correlated Materials" , (AIST-RIKEN), Okinawa , Mar. (2009).*
(8) Arima T.: “Neutron studies on magnetoelectric multiferroics”, Workshop on Possible Scientific View from New Neutron Spectroscopy Opportunities in J-PARC, Tokai, July (2009).
(9) Sagayama H., Abe N., Taniguchi K., Arima T., Yamasaki Y., Okuyama D., Tokura Y., Sakai S., Morita T., Komesu T., Ohsumi H., and Takata M.: “Observation of spin chirality using circularly-polarized synchrotron radiation X-rays”, 2009 Gordon Research Conference on X-Ray Science Waterville, USA, Aug. (2009).
(10) Arima T.: “Polarized neutron and synchrotron X-ray studies of helimagnetic ferroelectrics”, Polarized Neutrons and Synchrotron X-rays for Magnetism 2009, Bonn, Germany, Aug. (2009).*
(11) Arima T.: “X-ray study of magnetism in Sr2IrO4”, Workshop on POSTECH-RIKEN Joint Research Program, Sayo, Oct. (2009).
(12) Arima T., Abe N., and Taniguchi K.: “Domain-wall structures in cycloidal magnetoelectric multiferroics”, RIKEN Workshop on Emergent Phenomena of Correlated Materials, Wako, Dec. (2009).
(13) Fujiyama S., Kim B. J., Ohsumi H., Komesu T., Hirai D., Ohashi K., Sakai S., Arima T., and Takagi H.: "LS separation of J=1/2 Mott insulator observed by magnetic X-ray diffraction", American Physical Society 2009 March Meeting, Pittsburgh, USA, Mar. (2009).

(14) Arima T.: "Domain Control in Orbital-Ordered Systems", 2009AIST-RIKEN Joint WS Emergent Phenomena of Correlated Materials, Nago, Japan, Mar. (2009).
(15) Fujiyama S., Ohashi K., Ohsumi H., Sugimoto K., Arima T., and Takagi H.: "Magnetic structure of Sr3Ir2O7 determined by magnetic X-ray diffraction", 2009 RIKEN Workshop on Emergent Phenomena of Correlated Materials, Wako, Japan, Dec. (2009).
(16) Ohsumi H.: "Resonant X-ray magnetic scattering in 5d transition metal oxide", UK-Japan Meeting on Novel Quantum Phases in Oxide Materials, Bristol, UK, Feb. (2010).*
(17) Arima T., Ohsumi H., Takeshita S., Sagayama H., Okuyama D., Fujiyama S., Kim B. J., and Takagi H.: "Synchrotron X-ray as a Useful Probe for Frustrated Magnets", Highly Frustrated Magnetism 2010, Baltimore, MD, USA, Aug. (2010).*
(18) Yumoto H., Koyama T., Hirata K., Kawano Y., Ueno G., Nisawa A., Hikima T., Takeshita S., Ohsumi H., Ito K., Tanaka Y., Arima A., Ohashi H., Yamamoto M., and Goto S.: "Long working distance Kirkpatrick-Baez mirrors for hard X-ray beamlines at SPring-8", The 10th international conference on x-ray microscopy, Chicago, Illinois, USA, Aug. (2010).
(19) Ishiwata S., Kaneko Y., Tokunaga M., Okuyama D., Tokunaga Y., Arima T., Wakimoto S., Kakurai K., Taguchi Y., Tokura Y.: “Anomalous Hall effect in the helimagnetic cubic perovskite $SrFeO_3$”, Opening Symposium of QS2C Theory Forum, Wako, Japan, Sep. (2010).
(20) Arima T.: “Spin-induced polarization in triangular lattice”, Opening Symposium of QS2C Theory Forum, Wako, Japan, Sep. (2010).
(21) Yamaura J., Ohgushi K., Yamauchi I., Takigawa M., Hiroi Z., Ohsumi H., Sugimoto K., Takeshita S., Tokuda A., Arima T.: “Phase transition and magnetism in the pyrochlore oxide $Cd_2Os_2O_7$”, International conference on frustration in condensed matter, Sendai, Japan, Jan. (2011).
(22) Fujiyama S., Niitaka S., Ohsumi H., Takeshita S., Sugimoto K., Arima T., Takagi H.: “Metal-insulator transition in $(Pr_{1-x}Nd_x)_2Ir_2O_7$ and $(Pr_{1-x}Eu_x)_2Ir_2O_7$”, International conference on frustration in condensed matter, Sendai, Japan, Jan. (2011).
(23) Kanazawa N., Onose Y., Arima T., Okuyama D., Ohoyama K., Wakimoto S., Kakurai K., Ishiwata S., Tokura Y.: “Gigantic topological Hall effect in MnGe”, International conference on frustration in condensed matter, Sendai, Japan, Jan. (2011).

G. Future Plan

By utilizing the experimental techniques that we developed so far, we will study magnetic structures in various interesting systems in collaboration with active research groups. We also develop a new system to investigate the possible impact of electric current on spin texture by utilizing magnetic x-ray diffraction. The interplay between electric conduction and spin superstructure like a ferromagnetic domain wall is directly linked to a key technology in spin-electronic devices. A small focus of x-ray beam is a definite advantage for this purpose, because the density of the applied current can be much higher than in the case of neutron diffraction. We are now developing an x-ray microdiffraction system operating at low temperatures in collaboration with RIKEN SR Materials Science Instrumentation Unit and JASRI Optics Group. The combination of the polarization modulation technique with the scanning-type diffraction will enable us to detect various types of domains in ferroic materials. Within the present seven-year project, we will apply the scanning diffraction technique to the real-space imaging of static spatial distributions of such ferroic domains.

H. Curriculum Vitae (Team Leader)

NAME: Taka-hisa ARIMA

DATE OF BIRTH: October 10, 1963

EDUCATION:

1986: Graduated from Department of Applied Physics, University of Tokyo
1988: Master Degree from Department of Applied Physics, University of Tokyo

DEGREES: Ph.D (Science)

APPOINTMENTS:

1990-1991: JSPS Fellow
1991-1995: Research Associate, Department of Physics, University of Tokyo
1995-1995: Research Associate, Department of Applied Physics, University of Tokyo
1995-2004: Associate Professor, Institute of Materials Science, University of Tsukuba
2001-2007: Group Leader, ERATO-Spin Superstructure Project, JST
2004-2011: Professor, Institute of Multidisciplinary Research for Advanced Materials, Tohoku University
2011-: Professor, Department of Advanced Materials Science, University of Tokyo
2007-: Team Leader, Spin Order Research Team, Quantum Order Research Group, SPring-8 Center, RIKEN

ACADEMIC ACTIVITIES:

The Physical Society of Japan
The Japan Society of Applied Physics
The Japan Society of Neutron Science
The Japan Society of Synchrotron Radiation Research

1999: 日本物理学会論文賞

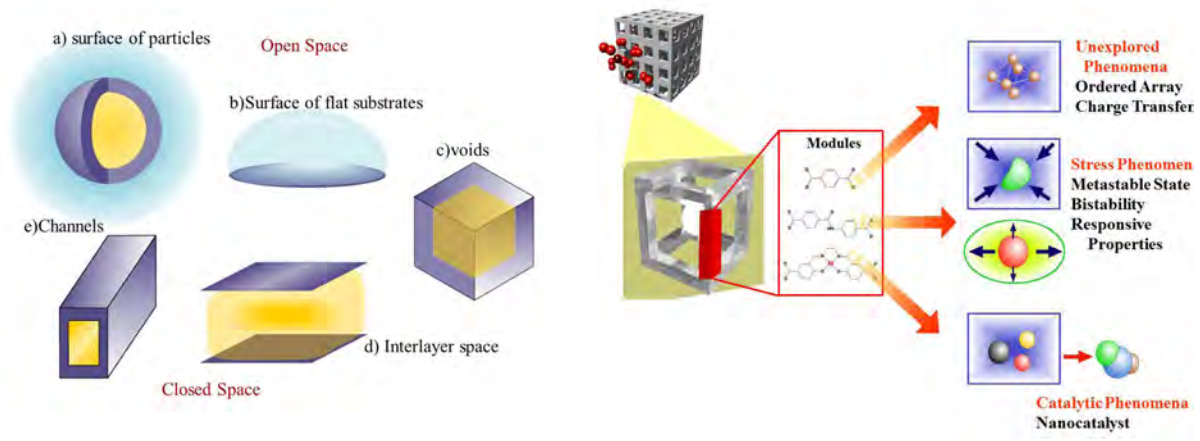
2-8-2. Spatial Order Research Team / 空間秩序チーム

Team Leader; Susumu Kitagawa, Dr. Eng. / 北川進
Since April 2007

A. Research Topics (Highlights)

1. Spatial Order Research Project

Remarkable progress has been made in the synthesis of coordination compounds with infinite structures, and in particular compounds with backbones constructed from metal ions as connectors and ligands as linkers, so-called coordination polymers (CPs). We have synthesized epoch-making space materials, visualizing sorption and desorption behaviors of guest molecules by crystallography and developing “exact science” of coordination space materials, which have a variety of functions. In nanospace built for energy storage and transfer, we can control and create chemical and physical functions such as charge separations and proton/electron transfers. Molecules and aggregates trapped in nanospace may have the potential to show physical properties based on quantum effects. This area is intended to focus on the scientific field from the new viewpoint (coordination space), which has not been seen in traditional chemistry and physics. We could define *coordination space* as those spaces where the coordination bond plays an important role in the formation of the spatial structures and where various physical properties are exhibited.



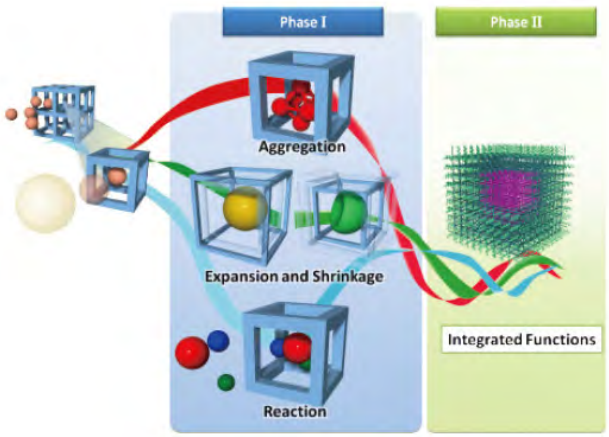
The mission in this field is to explore characteristics of the molecular systems in nanospace in the followings.

(1) new synthetic method to control nanosize space (nanospace) precisely
(2) various novel *Nanospace Materials*
(3) magnetic, dielectric and optical properties
(4) reactivity and catalytic functionality

In particular, we will focus on the unpredictable but key phenomena such as condensation of molecules, molecular stresses, and activation of molecules that may occur in these spaces. For this aim, we will develop a measurement system of quantum spatial order which makes full use of high luminosity of SPring-8. Moreover, cooperating other two teams, we reveal molecular interaction from spin order, excitation order and spatial order of electrons. We aim to pioneer material science with synchrotron radiation and find a new way to design bottom-up material especially.

2. Integrated Pore Project (ERATO)

To date PCPs are found in fledgling, 'Phase I' developments, in which pore functions are explored individually. Our aim of this project is to establish a symbiotic integration of porous materials and porous functions; hence, to develop PCPs with "controllable and flexible performance responsive to target environments", that is 'Phase II' developments. These environments range in size from the intermolecular or interatomic distances of the pores of materials (0.1-10 nm) up to the space inside biological cells (100 nm). Nonlinear, cooperative events taking place in mesospace present challenging problems and may hold the key to the technologies of tomorrow.



3. Clarification of Gas Adsorption Dynamics (XFEL)

We will visualize a gas adsorption process into nanopores of PCPs through diffraction and precision crystal structure analysis using an ultra high intensity XFEL light source and determine adsorption phenomena in terms of interaction between gas molecules and nanopores.

B. Research Subjects

(1) Investigation of expression systems of advanced material properties at time scale of pico second order
(2) Development of Porous Coordination Polymer with Pluripotent Pore/Hybrid Pore
(3) Visualization of gas adsorption process into nanopores of PCPs

C. Projects

Project name	Category	Started	Completed
Development of the Foundation for Nano-Interface Technology	JST, CREST	2006	2012
XFEL	MEXT, XFEL Research Promotion Program	2006	2010
Bilateral Joint Projects	MEXT Grant	2007	2009
ERATO Kitagawa Integrated Pores	JST, ERATO	2007	2013
NEDO Green and Sustainable Chemical Processes Project	NEDO Grant	2010	2011

D. Members

as of March 1st, 2011

	number	Name
Research Staff	2	Susumu Kitagawa, Akihiro Hori
Technical Scientist	0	

Research Staff	0	
Technical Staff	0	
Visiting Researchers	16	
Trainees	7	

E. Funding

(million yen)

	FY2008	FY2009	FY2010
Laboratory budget from RIKEN	21	23	18
Competitive fund in RIKEN			
Competitive fund outside RIKEN	0	0	0
Other fund from University, Private foundations etc.	0	0	0

F. Research Output

	FY2008	FY2009	FY2010
International Publications	6	4	5
Publications in Japanese	0	0	0
Oral Presentations	19	22	23
Patent Applications	0	0	0

a. Papers

(1) Tanaka D., Nakagawa K., Higuchi M., Horike S., Kubota Y., Kobayashi T., Takata M., Kitagawa S.: “Kinetic Gate-Opening Process in a Flexible Porous Coordination Polymer”, Angew. Chemi. Int. Ed. 47, 3914--3918 (2008).

(2) Comotti A., Bracco S., Sozzani P., Horike S., Matsuda R., Chen J., Takata M., Kubota Y., Kitagawa S.: “Nanochannels of Two Distinct Cross-Sections in a Porous Al-Based Coordination Polymer”, J. Am. Chem. Soc. 130, 13664--13672 (2008) .

(3) Zhang J. P., Kitagawa S.: "Supramolecular Isomerism, Framework Flexibility, Unsaturated Metal Center, and Porous Property of Ag(I)/Cu(I) 3,3’,5,5’- Tetrametyl-4, 4’- Bipyrazolates", J. Am. Chem. Soc. 130, 907-917 (2008).

(4) Ghosh S. K., Sareeya B., Kitagawa S.: "Dynamic Porous Coordination Polymer Functionalized by Isocyanurate", Angew. Chem. Int. Ed. (2008).

(5) Ohba M., Kaneko W., Kitagawa S., Maeda T., Mito M.: "Pressure Response of Three-dimensional Cyanide- bridged Bimetallic Magnets", Angew. Chem. Int. Ed. (2008).

(6) Ohba M., Yoneda K., Agusti G., Munoz M., Gaspar A., Real J., Yamasaki M., Ando H., Nakao Y., Sakaki S., and Kitagawa S.: "Bidirectional Chemo-Switching of Spin State in a Microporous Framework", Angew. Chem. Int. Ed. 48, 4767-4771 (2009).

(7) Agusti G., Ohtani R., Yoneda K., Gaspar A. B., Ohba M., Sanchez-Royo J., Munoz M., Kitagawa S., and Real J. A.: "Oxidative Addition of Halogens on Open Metal Sites in a Microporous Spin-Crossover Coordination Polymer", Angew. Chem. Int. Ed. 48, 8944-8947 (2009).

(8) Ohba M., Yoneda K., and Kitagawa S.: "Guest-Responsive Porous Magnetic Frameworks Using Polycyanometallates", CrystEngComm. 12, 159-165 (2009).

(9) Higuchi M., Tanaka D, Horike S, Sakamoto H, Nakamura K, Takashima Y, Hijikata Y, Yanai N, Kim J, Kato K, Kubota Y, Takata M. and Kitagawa S.: "Porous Coordination Polymer with Pyridinium Cationic Surface, $[Zn_2(tpa)_2(cpb)]$ ", J. Am. Chem. Soc. 131, 10336-10337 (2009).

(10) Shimomura S., Higuchi M., Matsuda R., Yoneda K., Hijikata Y., Kubota Y., Mita Y.,

Kim J., Takata M and Kitagawa S.: "Selective Sorption of Oxygen and Nitric Oxide by an Electron-Donating Flexible Porous Coordination Polymer", Nature Chemistry 2, 633-637 / (2010).

(11) Sato H., Matsuda R., Sugimoto K., Takata M. and Kitagawa S.: "Photoactivation of a Nanoporous Crystal for On-demand Guest Trapping and Conversion", Nature Materials 9, 661-666 (2010).

(12) Matsuda R., Tsujino T., Sato H., Kubota Y., Morishige K., Takata M. and Kitagawa S.: "Temperature Responsive Channel Uniformity Impacts on Highly Guest-Selective Adsorption in a Porous Coordination Polymer", Chemical Science 1, 315-321 (2010).

(13) Kato K., Hirose R., Takemoto M., Ha S., Kim J., Higuchi M., Matsuda R., Kitagawa S. and Takata M.: "The RIKEN Materials Science Beamline at SPring-8: Towards Visualization of Electrostatic Interaction", AIP conference Proceedings 1234, 875-878 (2010).

(14) Fukushima T., Horike S., Inubushi Y., Nakagawa K., Kubota Y., Takata M. and Kitagawa S.: "Solid Solutions of Soft Porous Coordination Polymers: Fine-Tuning of Gas Adsorption Properties", Angew. Chem. Int. Ed. 49, 4820-4824 (2010).

b. Oral Presentations (* Invited presentation)

listed only plenary lecture by Prof. Susumu Kitagawa

(1) “New Aspects of Porous Coordination Polymers”, 10th Eurasia Conference on Chemical Sciences (EuAsC_2S-10), Manila, Philippines, Jan. (2008)*

(2) “Porous Coordination Polymers”, meeting at the TUDelft on MOFs (or coordination polymers), Kingdom of the Netherlands, Jan. (2008)*

(3) “Design and Functions of Porous Coordination Polymers”, ISNNM 2008, The Gyeongju TEMF Hotel, Gyeongju, Korea, May (2008)*

(4) “Soft Porous Crystals of Coordination Polymers”, 4th EuCheMS Conference on Nitrogen Ligands in Coordination Chemistry, Garmisch-Partenkirchen, Germany, Aug. (2008)*

(5) “New Aspects of Porous Coordination Polymers”, The 11th International Conference on Molecule Based Magnets (ICMM 2008), Florence, Italy, Sept. (2008)*

(6) “Chemistry and Applications of Soft Porous Crystals”, 5th Host-Guest Chemistry Symposium, Utsunomiya University, Utsunomiya, Japan, May (2009)*

(7) “Responsive Properties of Porous Coordination Polymers”, The 19th edition of the International Conference on the Chemistry of the Organic Solid State (ICCOSS XIX), Sestri Levante, Genova, Italy, June (2009)*

(8) “Coordination Polymers Having Integrated Pores”, MOFCAT 2009 Workshop, Oslo, Norway, June (2009)*

(9) “Porous Coordination Polymers”, RSC Coordination Chemistry Discussion Group Annual Meeting, Leeds, UK, June (2009)*

(10) “Dynamic Behavior of Gas and Polymer Molecules Confined in Porous Coordination Solids”, 6th National Conference on Coordination Chemistry (cum International Symposium on Coordination Chemistry), Hong Kong, China, July (2009)*

(11) **“**Chemistry and Application of Porous Coordination Polymers”, The International Symposium on Zeolites and Microporous Crystals (ZMPC2009), Waseda University, Tokyo, Japan, Aug. (2009)*

(12) “Chemistry of Porous Coordination Polymers”, 31st International Conference on Solution Chemistry (ICSC 2009), Innsbruck, Austria, Aug. (2009)*

(13) “Soft porous crystals from porous coordination polymers”, The XXXIInd Annual British Zeolite Association Conference, University of Cumbria, Ambleside, Aug. (2009)*

(14) “Perspectives of porous coordination polymers”, Sino-German Workshop "Designed Materials for Energy Related Catalytic Processes", Dalian, China, Sept. (2009)*
(15) “Chemistry and Applications of Soft Porous Crystals”, The 15th Chinese Zeolite Conference (15th CZC), Luoyang, Henan, China, Oct. (2009)*
(16) “Functions of Soft Porous Coordination Polymer Crystals”, 61st Southeastern Regional Meeting of the ACS (SERMACS 2009), San Juan, Puerto Rico, Oct. (2009)*
(17) “Perspectives of porous coordination polymers”, Symposium on Modern Trend in Inorganic Chemistry (MTIC-XIII), Bangalore, India, Dec. (2009)*
(18) “Soft Porous Coordination Polymers”, Nanomaterials and Functionality, Valencia, Spain, May (2010)*
(19) “Integrated Pores and Multifunctionalities of Porous Coordination Polymers”, MOLMAT 2010, Montpellier, France, July (2010)*
(20) “Coordination Polymers with Integrated Functional Pores”, International Symposium on Advancing the Chemical Science-Challenges in Inorganic and Materials Chemistry (ISACS3), Hong Kong, China, July (2010)*
(21) “Evolution of Porous Coordination Polymers”, 39th International Conference on Coordination Chemistry (ICCC39), Adelaide, South Australia, July (2010)*

G. Future Plan

Recently a huge number of PCPs have been reported. PCPs can exhibit some superior functions such as in storage, catalysis and highly enantio-, size- and shape-selective adsorption. The performance of PCPs has been improving as the result of trial and error, however rational molecular design based on detailed analysis of host-guest interaction is undeveloped so far. In our perspectives, our major goal is the development of new space materials with rational design for desired functions. For this purpose, we will synthesize organic linkers, create novel PCPs, and thoroughly utilize synchrotron X-ray beam to elucidate the origin of their function. The function of their pore will be explored by using Maximum Entropy Method and Rietveld analysis, which will be feed back to the molecular design. In addition, we are interested in an interaction force between adsorbed molecules and/or the pore walls and in sorption dynamics, especially short-live intermediate phase and adsorption process. Therefore, we will develop simultaneous measurement system of the Raman spectroscopy and the gas sorption. This is an original system and make also applicable for the diffraction measurement at BL44B2 site, which makes it possible to obtain triplicate data, Raman spectrum, adsorption isotherm and data diffraction, simultaneously. In addition, the experimental electrostatic potential analysis will visualize molecular interaction. The multidimensional analyses will reveal essential features of PCPs from macroscopic to nanoscopic scale. Also we will try to deliver precise on-demand control of the functions of space materials using external stimuli, e.g. light, magnetic field, electric field, which will be dramatically promoted through inter-team collaboration with spin order and excitation order research teams.

H. Curriculum Vitae (Team Leader)

NAME: Susumu KITAGAWA

DATE OF BIRTH: July 4, 1951, Kyoto, Japan

EDUCATION:

1971-1974	Kyoto University, Kyoto, Japan Undergraduate course, Hydrocarbon Chemistry
1975-1979	Kyoto University, Kyoto, Japan Graduate School, Hydrocarbon Chemistry

ACADEMIC DEGREES: Ph.D.

APPOINTMENTS:

1979-1983	Assistant Professor, Kinki University, Higashi-Osaka, Japan Department of Chemistry
1983-1988	Lecturer, Kinki University, Higashi-Osaka, Japan Department of Chemistry
1986-1987	Visiting Scientist, Department of Chemsitry, Texas A & M University F.A.Cotton Laboratory
1988-1992	Associate Professor, Kinki University, Higashi-Osaka, Japan Department of Chemistry
1992-1998	Professor, Tokyo Metropolitan University, Hachiouji, Tokyo, Japan Department of Chemistry
1998-	Professor, Kyoto University, Kyoto, Japan Department of Synthetic Chemistry & Biological Chemistry
2004 -2007	Leader of MEXT Grant; Priority Area, “Chemistry of Coordination Space”
2007 -	Deputy Director, Institute for Integrated Cell-Material Sciences, Kyoto University
2007-2013	Leader of ERATO program, “Integrated Pores”

ACADEMIC ACTIVITIES:

2001-2002	Vice-president, Japanese Society of Coordination Chemistry
2004 -	Editor for *Chemistry Letters*, Topic Editor for *Crystal Growth & Design*
2006 -	Editor for *Chemical Communications*, *Chemistry - Asian Journal*, *Chemistry of Materials*, *Inorganica Chimica Acta*, *Coordination Chemistry Reviews*, *CrystEngComm*, *European Journal of Inorganic Chemistry*
2008-	Asian Editor for *ChemEngComm*, *Inorganic Chemistry*

2-8-3. Excitation Order Research Team / 励起秩序研究チーム

Team Leader; Shik SHIN, Dr. Sci. / 辛　埴
Since April 2007

A. Research Topics (Highlights)

1. Study of chirality by Resonant soft X-ray diffraction

We have successfully developed a new experimental tool to determine the absolute crystal chirality by using resonant x-ray diffraction of circularly polarized x-rays. Chirality, or handedness, is ubiquitous in life at all length-scales, down to individual molecules. An object is said to be chiral if there is no mirror reflection that leaves the object unchanged. Given the close relationship between diffraction and symmetry, it might seem surprising that the most basic and well-understood mechanism responsible for X-ray diffraction, the standard tool for studies of crystal symmetry, cannot distinguish between left- and right-handed structures. However, since the seminal paper by Bijvoet in 1951, researchers have known how to extract chiral information from the small differences in the intensity of sister reflections called 'Friedel pairs' by exploiting the proximity of atomic resonances in the materials under investigation. That technique relies on a careful analysis of interference between the waves scattered from various types of atom in the target crystal. Our method is quite different from this. We use circularly polarized x-rays at certain energies, or absorption edges.

Berlinite ($AlPO_4$) and low-quartz (SiO_2) have enantiomers belonging to a space-group pair, $P3_121$ (right-handed screw) and $P3_221$ (left-handed screw). We use circularly polarized resonant x-ray diffraction to study structural chirality. Our results demonstrate that positive and negative circularly polarized x-ray diffraction at the resonant energy of berlinite (Al 1s edge) and low-quartz Si (1s edge) can distinguish the absolute structure (right or left-handed screw) of an enantiomer. The azimuth scans for *L* berlinite observed at the resonant energy *E*=1566.8 eV, where the intensity of the diffracted beam is the maximum, together with the data for *L* quartz measured at *E*=1847.9 eV. Clearly the intensity of the diffracted beam changes with helicity of the x-ray beam. The advantage of our method is that the measurement of only one space-group forbidden reflection is enough to determine the chirality. This method is applicable to chiral motifs that occur in biomolecules, liquid crystals, ferro- and antiferro-electrics, multiferroics, etc. [Y. Tanaka *et al*., Phys. Rev. Lett., **100**, 145502 (2008), Phys. Rev. B**81**, 14410 (2010)]

2. Exploring the study of liquids by soft X-ray emission spectroscopy

The electronic structure of a material is important for many fields of science, because valence electrons play important roles in determining material properties. In aqueous solution, molecules are considered to have particular interaction with surrounding molecules in a different state from solid or gas phase. Hence, observations of the electronic structure of molecule in aqueous solution will bring direct and fascinating information for their properties. Owing to developments of experimental techniques, electronic structures of liquids and solutions have become accessible recently. One of these experimental techniques is the x-ray emission spectroscopy using synchrotron radiation light source.

Among the liquids, liquid water is unusual in that it shows many anomalies in its thermodynamic properties such as compressibility, density variation and heat capacity. Recently, we found interesting and unexpected results in x-ray emission spectra of water using liquid flow cell developed by us at SPring-8 BL17SU. What we found was clear peak

splitting in lone-pair orbital region which had not been observed in previous reports of Guo et al. in 2002, due to limitation of energy resolution. To investigate the origin of these two peaks of lone-pair orbital region, the XES spectra of water in three states (gas, liquid, solid) and temperature dependence of liquid water was studied. These results lead us to interpret the two peaks as representing tetrahedral-like and highly distorted structural motifs, providing evidence against an unstructured continuum model of the liquid which had been believed over 60 years. [T. Tokushima *et al*., Chem. Phys. Lett., **460**, 387 (2008)]

Combined the experimental results of SAXS and XES, we propose that the contrast of density difference in SAXS is due to fluctuations between tetrahedral ice-like and hydrogen-bond distorted structures related to, respectively, low and high density water. The results of our present studies which indicate presence of density fluctuations in ambient water on a physical length-scale around 1 nm. [C. Huang *et. al*., PNAS **106**, 15214 (2009)]

Another aspect we obtained recently is concerning about solute molecule in solution, which seems to be important especially for chemistry than our results on pure water as shown above. We studied the electronic structure of acetic acid molecules in aqueous solutions. Acetic acid is a simple and common acid containing a single carboxyl group (-COOH). Acetic acid represents a model case to discuss deprotonation causing the neutral to anionic transition. Hence, it is important to study the occupied valence electronic structure of solutions in acid-base equilibrium.

These results indicated that the two states of acetic acid did not interact with each other; instead, each state was static and stable, with populations determined by the solution pH. The unexpected perfect match between the ratio analysis of the XES spectra and a static acid–base equilibrium equation indicate that water molecules stabilize the acetic acid states, possibly by hydration around the acid molecules.

3. Photoemission study of surface adsorbtes and thin films

In collaboration with Kawai laboratories in RIKEN and Univ. Tokyo, adsorption-induced switching of magnetic anisotropy was found in Iron (II) phthalocyanine (FePc) on oxidized Cu (110) surface by high-resolution photoemission spectroscopy and inelastic electron tunneling spectroscopy. The Fe 2p core level photoemission spectra revealed that the spin state converts from triplet in FePc/O/Cu (110) to singlet in FePc/clean-Cu (110). The finding demonstrates the importance of coupling at the molecular-substrate interface for manipulating the magnetic properties of adsorbates. [Tsukahara *et al*., Phys. Rev. Lett.**102**, 167203 (2009)]

We have also succeeded in mapping Fermi-surface (FS) of epitaxial ultrathin Fe films on fcc Cu (001). The 8 monolayer thin film exhibits a spin spiral (SS) in contrast to the ferromagnetism of bulk bcc Fe. In-plane (IP) and out-of-plane (OP) FSs were obtained by the energy-dependent soft-x-ray momentum-resolved photoemission. It was revealed that the SS originates in nested regions confined to OP FSs, which are drastically modified compared to IP FSs. Furthermore, from precise reciprocal-space maps in successive zones, we obtain the associated real space compressive strain of 1.5% along c axis. The results reveal the importance of IP and OP FS mapping for ultrathin films. [Miyawaki *et al*., Phys. Rev. Lett.**104**, 066407 (2010)]

B. Research Subjects

(1) Soft X-ray and hard X-ray photoemission spectroscopy on strongly correlated materials
(2) Soft X-ray emission spectroscopy on liquids and biomaterials
(3) Soft X-ray emission and photoemission spectroscopy on Surface and interface

C. Projects

Project name	Category	Started	Completed
Nano-scale Science & Technology	Institute Program	2007	2011
Hydration Dynamics and Molecular Process	Institute Program	2007	2010
Molecular Ensemble	Institute Program	2006	2011
Research and Development of Soft X-ray Diffraction for Structural Chirality	Institute Program	2008	2010
Complex Electron Systems	Institute Program	2005	2009
Development for Soft X-ray Resonant Diffraction under High Magnetic Field	MEXT, Grant-in-Aid for Scientific Research (A)	2009	2011
Research on Self-organization for Advanced Materials with Novel Electric Functions	MEXT, Grant-in-Aid for Creative Scientific Research	2004	2008
Transformative Research-project on Iron Pnictides	JST, TRIP	2008	2012

D. Members

as of March 1st, 2011

	number	Name
Research Scientist	9	Shik Shin, Yasutaka Takata, Ashish Chainani, Yoshikazu Tanaka, Munetaka Taguchi, Takashi Tokushima, Jun Miyawaki, Takumi Ohtsuki, Yuka Horikawa
Technical Scientist	0	
Research Staff	0	
Technical Staff	0	
Visiting Researchers	34	
Trainees	14	

E. Funding

(million yen)

	FY2008	FY2009	FY2010
Laboratory budget from RIKEN	5	6	4
Competitive fund in RIKEN	33	61	41
Competitive fund outside RIKEN	29	30	1
Other fund from University, Private foundations etc.			

F. Research Output

	FY2008	FY2009	FY2010
International Publications	29	24	16
Publications in Japanese	4	2	14

Oral Presentations	68	55	44
Patent Applications	0	0	0

a. Papers

(1) Matsunami M., Eguchi R., Kisu T., Horiba K., Chainani A. A., Taguchi M., Yamamoto K., Togashi T., Watanabe S., Wang X. Y., Chen C. T., Senba Y., Ohashi H., Sugawara H., Sato H., Harima H., and Shin S.: "Anomalous duality of 4f electrons in filled skutterudite $CeOs_4Sb_{12}$", Phys. Rev. Lett. **102**, 036403-1-036403-4 (2009).

(2) Sugiura K., Ohta H., Ishida Y., Huang R., Saito T., Ikuhara Y., Nomura K., Hosono H., and Koumoto K.: "Structural transformation of Ca-arrangements and carrier transport properties in $Ca_{0.33}CoO_2$ epitaxial films", Appl. Phys. Express **2**, 035503-1-035503-3 (2009).

(3) Takeuchi T., Chainani A. A., Takata Y., Tanaka Y., Oura M., Tsubota M., Senba Y., Ohashi H., Mochiku T., Hirata K., and Shin S.: "An ultrahigh-vacuum apparatus for resonant diffraction experiments using soft x rays (hv=300-2000 eV)", Rev. Sci. Instrum. 80, 023905-1-023905-7 (2009).

(4) Sugiura K., Ohta H., Ishida Y., Huang R., Saito T., Ikuhara Y., Nomura K., Hosono H., and Koumoto K.: "Structural transformation of Ca-arrangements and carrier transport properties in $Ca_{0.33}CoO_2$ epitaxial films", Appl. Phys. Express **2**, pp035503-1-035503-3 (2009).

(5) Eguchi R., Okamoto Y., Hiroi Z., Shin S., Chainani A. A., Tanaka Y., Matsunami M., Takata Y., Nishino Y., Tamasaku K., Yabashi M., and Ishikawa T.: "Structure and photoemission spectroscopy of strain-controlled metal-insulator transition in $NdNiO_3$ thin films", J. Appl. Phys. **105**, pp056103-1-056103-3 (2009).

(6) Harada Y., Taguchi M., Miyajima Y., Tokushima T., Horikawa Y., Chainani A. A., Shiro Y., Senba Y., Ohashi H., Fukuyama H., and Shin S.: "Ligand energy controls the heme-Fe valence in aqueous myoglobins", J. Phys. Soc. Jpn. **78**, No.4, pp044802-1-044802-5 (2009).

(7) Horikawa Y., Tokushima T., Harada Y., Takahashi O., Chainani A. A., Senba Y., Ohashi H., Hiraya A., and Shin S.: "Identification of valence electronic states of aqueous acetic acid in acid-base equilibrium using-selective x-ray emission spectroscopy", Phys. Chem. Chem. Phys. **11**, No.39, pp8676-8679 (2009).

(8) Tokushima T., Horikawa Y., Harada Y., Takahashi O., Hiraya A., and Shin S.: "Selective observation of the two oxygen atoms at different sites in the carboxyl group (-COOH) of liquid acetic acid", Phys. Chem. Chem. Phys. **11**, pp1679-1682 (2009).

(9) Mulazzi M., Miyawaki J., Chainani A. A., Takata Y., Taguchi M., Oura M., Senba Y., Ohashi H., and Shin S.: "Fermi surface of Co(0001) and initial-state linewidths determined by soft x-ray angle-resolved photoemission spectroscopy", Phys. Rev. B **80**, pp241106-1-241106-4 (2009).

(10) Huang C., Wikfeldt K., Tokushima T., Nordlund D., Harada Y., Bergmann U., Niebuhr M., Weiss T. M.,Horikawa Y., Leetmaa M., Ljungberg M. P., Takahashi O., Lenz A., Ojamae L., Lyubartsev A. P., Shin S., Pettersson L. G., and Nilsson A.: "The inhomogeneous structure of water at ambient conditions", Proc. Natl. Acad. Sci. USA **106**, No.36, pp15214-15218 (2009).

(11) Miyawaki J., Chainani A. A., Takata Y., Mulazzi M., Oura M., Senba Y., Ohashi H., and Shin S.: "Out-of plane nesting driven spin spiral in ultrathin Fe/Cu(001) films", Phys. Rev. Lett. **104**, pp066407-1-066407-4 (2010).

(12) Taguchi M., Chainani A., Matsunami M.,Eguchi R., Takata Y., Yabashi M., Tamasaku K., Nishino Y., Ishikawa T., Takagi H., and Shin S.: "Anomalous State Sandwiched between Fermi Liquid and Charge Ordered Mott-Insulating Phases of Ti_4O_7", Phys. Rev. Lett. **104**, pp106401-1-106401-4 (2010).

(13) Tokushima T., Harada Y., Horikawa Y., Takahashi O., Senba Y., Ohashi H., Pettersson L. M., Nilsson A., Shin S.: "High resolution x-ray emission spectroscopy of water and its assignment based on two structural motifs", J. Electron. Spectrosc. Relat. Phenom. **177**, 192-205 (2010)..

(14) Horikawa Y., Tokushima T., Hirata A., Shin S.: "Pronounced polarization anisotropy in resonant x-ray emission from acetic acid molecules in solution", Phys.Chem.Chem.Phys.

12, 9165-9168（2010）.
(15) Okawa M., Matsunami M., Ishizaka K., Eguchi R., Taguchi M., Chainani A. A., Takata Y., Yabashi M., Tamasaku K., Nishino Y., Ishikawa T., Kuga K., Horie N., Nakatsuji S., Shin S.: "Strong valence fluctuation in the quantum critical heavy fermion superconductor β-$YbAlB_4$: a hard x-ray photoemission study", Phys Rev. Lett. **104**, 247201- 1-247201-4（2010）.
(16) Ohtsuki T., Chainani A., Eguchi R., Matsunami M., Takata Y., Taguchi M., Nishino Y.,Tamasaki K., Yabashi M., Ishikawa T., Oura M., Senba Y., Ohashi H., Shin S.,: "Role of Ti 3*d* carriers in mediating the ferromagnetism of Co:TiO_2 anatase thin films", Phys Rev. Lett., **106**, 047602-1-047602-4 (2011)

b. Oral Presentations (* Invited presentation)

(1) Shin S., "Inelastic soft x-ray scattering of protein and amino acids in water", Resonant Inelastic Soft X-Ray Scattering Workshop (RIXS09), Grenoble, France (2009)
(2) Takata Y., "Hard x-ray photoelectron spectroscopy", 11th International Conference on Electronic Spectroscopy and Structure, Nara, Japan (2009)
(3) Shin S., "Hard x-ray photoelectron spectroscopy", The 10th International Conference on Synchrotron Radiation Instrumentation, Melbourne, Australia (2009)
(4) Takata Y., "Hard x-ray photoelectron spectroscopy", The 37th international conference on vacuum ultraviolet and x-ray physics (VUVX1010), Univ. British Columbia, Vancouver, Canada (2010)

G. Future Plan

We will continuously improve and develop spectroscopies, and will extend its application to new material science in collaboration with RIKEN researchers, other Institutes as well as University groups.

1) Utilization of newly developed SX spectroscopies

- The present SX- and HX-PES systems have the highest resolutions of the world. However, the resolution of PES is still not enough to discuss physics of materials below an energy scale of 50 meV. If we can achieve a 10-meV resolution, it would open up several new themes of research such as the gap behaviour in high-temperature superconductors, Kondo scale studies in f-electron systems, etc. It is hence important to upgrade the photoemission resolution.
- Recently, the resolution of the SXES has significantly improved in SLS and ESRF. We also know of plans to construct new SXES spectrometers at other foreign SR facilities. In order to compete with the SXES groups worldwide, we must construct a new SXES spectrometer. This kind of ultra-high resolution spectroscopy should be one of the most important subjects for the SPring-8 II project.

2) Development of new materials science

Another important mission in the future is to develop new fields of materials science using various cutting-edge SX spectroscopies. Especially, the electronic structures of (1) liquids, (2) biomaterials, and (3) interfaces on solids are considered to be very important. We believe that we will be able to create important fields in future materials sciences. In particular, electronic structure of biomaterials will give fruitful information on their functions. We have started to use soft X-ray emission (SXE) spectroscopy as a new tool to investigate unique functions of biological samples, in collaboration with biology groups and materials science groups. .

H. Curriculum Vitae (Team Leader)

NAME: Shik SHIN

DATE OF BIRTH: July 7, 1953

EDUCATION:

1977: Department of Physics, Faculty of Science, The University of Tokyo
1980: Master Degree from Department of Physics, Faculty of Science, The University of Tokyo
1983: Dr. Science from Department of Physics, Faculty of Science, The University of Tokyo

DEGREES: Dr. Science

APPOINTMENTS:

1983-1989	Research associate of Research institute of measurement, Tohoku University
1989-1991	Associate professor of Research institute of measurement, Tohoku University
1991-2000	Associate professor of Institute for solid state physics, The University of Tokyo
1999-2007	Chief scientist, RIKEN
2000-	Professor of Institute for solid state physics, The University of Tokyo
2007-	Team leader, Excitation order Research Team, RIKEN

ACADEMIC ACTIVITIES:

Member of physical society of Japan
Editor of physical society of Japan
Member of Japanese society for synchrotron radiation research
Councilor of Japanese society for synchrotron radiation research
Member of Solid State Ionic

2-9. Song Initiative Research Unit / Song 独立主幹研究ユニット

Initiative Research Scientist; Changyong SONG, Ph. D/ 宋 昌容
Since March 2008

A. Research Topics (Highlights)

1. **Coherent X-ray diffraction tomography**
   The research has been focused on developing coherent X-ray diffraction imaging (CDI) technique for its application in 3D imaging of biological specimens and functional nano-structures. For the last several years, we have advanced essential techniques including robust phase-retrieval algorithms, 3D computer tomography methods and established adaptable X-ray diffraction imaging chamber. With the developments, we have successfully applied the technique to unravel 3D architecture of mammalian nuclei with detailed substructures better than 50 nm 3D image resolution. The work foreshadows new paradigm as a next generation genomics study – genomes in 3D – with CXDT. Presently we are working to realize cryo-CDI by implementing a cryogenic sample mounting system.

2. **FEL single-shot diffractive imaging**
   This projects aims to establish a methodology for single-particle 3D imaging by using intense, short pulse X-ray LASER lights produced by X-ray Free Electron Laser (XFEL). We have carried out various proof-of-concept experiments by using out prototype EUV-FEL facility at SCSS demonstrating the feasibility of single-shot diffractive imaging. Single-shot diffraction imaging of bio-molecular specimens, nano-particle embedded polymers and carbon nanotubes – mounted on fixed sample holders – has been successfully carried out. We are now developing single-particle injectors to accomplish single-molecule 3D imaging with our XFEL.

B. Research Subjects

(1) Coherent X-ray diffraction tomography
(2) XFEL single-particle 3D imaging
(3) Developing imaging methodology by using coherent X-rays

C. Projects

Project name	Category	Started	Completed
FEL & X-ray single-particle 3D imaging	MEXT : Grants-in-Aid for Science Research	04.2010	03.2012
Single-particle 3D reconstruction with EUV-FEL diffractive imaging	RIKEN President's Strategic Research Program for R&D	10.2008	09.2010

D. Members

as of March 1st, 2011

	Number	Name
Research Scientist	3	Changyong Song, Jaehyun Park, Sunam Kim
Technical Scientist	0	
Research Staff	0	
Technical Staff	1	Hiroki Shimada
Visiting Researchers	4	
Trainees	5	

E. Funding

(million yen)

	FY2008	FY2009	FY2010
Laboratory budget from RIKEN	39	39	39
Competitive fund in RIKEN	4	6	3
Competitive fund outside RIKEN	0	0	9
Other fund from University, Private foundations etc.	0	0	0

F. Research Output

	FY2008	FY2009	FY2010
International Publications	1	0	3
Publications in Japanese	0	0	0
Oral Presentations	1	3	7
Patent Applications	0	0	0

a. Papers

(1) Xu R., Salha S., Raines K., Jiang H., Chen C.-C., Takahashi,Y., Kohmura Y., Nishino Y., Song C., Ishikawa T., and Miao J.:
" Coherent diffraction microscopy at SPring-8: instrumentation, data acquisition and data analysis", J. Synchrotron Rad. 18, 293 (2011)

(2) Jiang H., Song C., Chen C.-C., Xu R., Raines K., Fahimian B., Lu C.-H., Lee T.-K., Nakashima A., Urano J., Ishikawa T., Tamanoi F., and Miao J.:
"Quantitative 3D imaging of whole, unstained cells by using X-ray diffraction microscopy", Proc. Natl. Acad. Sci. USA, 107, 11234 (2010)

(3) Park J., Kohmura Y., and Song C.:
"EUV-FEL diffraction imaging of nanostructures at SCSS", J. of the Jap. Soc. for Synchrotron Rad. Res. 23, 325 (2010)

(4) Song C., Jiang H., Mancuso A. P., Amirbekian B., Peng L., Sun R., Shah S. S., Zhou Z. H., Ishikawa T., and Miao J.:
"Quantitative imaging of single, unstained viruses with coherent X-rays", Phys. Rev.

Lett., 101, 158101 (2008)

b. Oral Presentations (* Invited presentation)

(1) Song C.; “Nano-scale Resolution 3D Imaging with Coherent X-ray Diffraction Microscopy”, Workshop on Neutron and X-ray Scattering for Structures and Dynamics of Nanoscale Materials, KAIST, Daejeon, Korea, Dec. (2010)*
(2) Song C.; “Coherent X-ray Imaging of Biological Specimens at SPring-8”, LCLS/SLAC Users Meeting, Workshop Frontiers in Biology with X-FELs, SLAC, Palo Alto, Oct (2010) *
(3) Song C.; “Toward Single-Macromolecule 3D Imaging with Intense, Short-Pulse X-ray Lasers”, Iowa State University, Oct. (2010)*
(4) Song C.; “Biological 3D Imaging with Coherent X-rays”, The 3rd International Workshop on FEL Science: “Emerging X-ray Applications in Biological Systems-II”, Hokkaido, Japan, Oct. (2010) *
(5) Song C.; “Diffractive Imaging of Biological Specimens with Intense, Coherent X-rays”, BE/OPT Workshop on X-FEL and Its Applications, Athens, Greece, June (2010) *
(6) Song C.; “Biological 3D imaging with Intense, Coherent X-rays”, Workshop on Coherent X-ray Imaging for Biological Applications at NSLS-II, Brookhaven, USA, May (2010) *.
(7) Song C.; “X-ray Diffraction Imaging at SPring-8”, APS-ESRF-SPring8 Three Way Meeting, SPring-8, Japan, April (2010) *.
(8) Song C.; “Diffractive Imaging with Coherent X-rays”, The 2nd International Workshop on FEL Science: “Emerging X-ray Applications in Biological Systems”, Kenting, Taiwan, December (2009) *.
(9) Song C.; “Toward Single -Macromolecule 3D Imaging with Intense, Short-Pulse X-ray Lasers”, The 10th International Conference on Synchrotron Radiation Instrumentation, Session: Hot Topics & Emerging Talents, Melbourne, Australia, October (2009) *.
(10) Song C.; “Toward Single -Macromolecule 3D Imaging with Intense, Short-Pulse X-ray Lasers”, The 1st International Workshop on FEL Science: “Coherent Intense X-rays in Physics and Biology”, Jeju, Korea, February (2009) *.
(11) Song C.; “Single Molecule 3D Imaging with Coherent Diffraction Microscopy”, The 30th International Free Electron Laser Workshop, Special Session, Korea, August (2008) *.

G. Future Plan

(1) Coherent X-ray diffraction tomography

We are planning to introduce cryo-CXDT by developing cryo-cooled sample stages and accompanied sample preparation protocols. This expects to establish CXDT as a practical biological imaging probe by its capability to image a specimen in hydrated state close to its native environment. With cryo-cooling we aim to achieve several nm scale 3D resolution. Further we are working to establish protein-specific imaging by implementing the immuno nano-particle labeling technique to CDI. It will realize studying protein-protein interaction *in situ.* Developed techniques will find good applications in *3D in situ genomics,* for instance.

(2) XFEL single-particle 3D imaging

With the pledged goal to accomplished single-particle 3D imaging at near atomic resolution with XFEL, we are developing relevant methodologies as well as apparatus. Various types

of single-particle injectors are currently under development to load fresh specimens either in liquid or vacuum ambiance compatible with our XFEL. Single-particle analysis algorithms are developed through collaborations. We aim to establish single-particle 3D imaging method in the modality of coherent x-ray diffraction imaging by fully utilizing the XFEL. Its practical applications to reveal 3D structures of macro-molecular complexes without crystallizations are much anticipated.

(3) Developing imaging methodology by using coherent X-rays

Further we plan to explore various new possibilities of imaging with coherent X-rays. Current there are certain limitations in applying the technique to resolve debating scientific issues explicitly. We will explore the polarization characteristics of X-ray and element/orbital-specific resonance property while interacting with specimens to realize analytic imaging probe. This will find broad applications in studying correlated electron materials as well as multi-color imaging of biological specimens.

H. Curriculum Vitae (Initiative Research Scientist)

NAME: Changyong SONG

DATE OF BIRTH: 5 May 1972

EDUCATION:

2001: Ph. D. Condensed Matter Physics, Iowa State University (Ames, USA)
1995: B.S. Physics, Jeonbuk National University (Jeonju, Korea)

ACADEMIC DEGREES:

Ph. D. Experimental condensed matter physics
B.S. Physics

APPOINTMENTS:

2008.03 - Present: Initiative Research Scientist, RIKEN
2010.04 - Present: Adjunct Professor, Physics, POSTECH
2004.12 - 2008.02: Post-Doc., UCLA
2001.04 - 2004.11: POSTECH, Post-Doc
1996.08 - 2001.03: Graduate Research Assistant, Ames Lab.-US.DOE

ACADEMIC ACTIVITIES:

Organizational Activities

2008, 2009, 2010: International Workshop on FEL Science

3. Advanced Photon Technology Division

3-1. Research Infrastructure Group / 基盤研究部

Group Director; Masaki Yamamoto, Ph D. / 山本 雅貴
Since November 2008

A. Outline of Research Infrastructure Group

Research Infrastructure Group is launched to explore the best use of the high-brilliant SR sources of SPring-8 and XFEL for various scientific fields such as materials science, life science, etc., through the research and development on new technologies and instruments at SPring-8 RIKEN beamlines. The R&D targets of our group are creating the new scientific field with the high-brilliant SR and improving the usability of SPring-8 beamlines. Direct observation of the transient phenomena in nano-scale and remote access from distinct users are the typical examples.

The group is responsible for managing the procedure of the research projects conducted at RIKEN beamlines, including a call for proposals, technical reviews and the experimental reports. The group consists of four units, SR Life Science Instrumentation unit, SR Materials Science Instrumentation unit, Soft X-ray Spectroscopy Instrumentation unit and SR Imaging Instrumentation unit. Each unit is responsible for research and development of advanced technology and methodology utilized in the various fields of SR science, as well as operations and user supports of eight RIKEN beamlines. The beamlines are BL26B1, BL26B2, BL32XU, BL45XU, BL17SU, BL19LXU, BL29XUL, and BL44B2, and the details are shown below.

RIKEN beamlines started with the configuration of four beamlines for biology and three for physics. The role of each beamline has been changed and upgraded as time goes on: Main subject of BL45XU has been shifted from protein crystallography to small angle scattering on soft matter including biological macromolecules. BL44B2 was switched to a materials science beamline from a protein crystallography beamline. At BL26B1 and B2, robotics technology has been applied to the sample changer system to achieve high-throughput structure analysis of protein crystals. Targeted protein beamline, BL32XU had been constructed and started user operation in May 2010 in order to create protein micro crystallography. As for the physics beamlines, all of them have special properties: BL29XUL has a 1 km-long beamline: BL19LXU has a 27 m-long undulator: BL17SU produces a coherent soft X-ray beam to give high energy-resolution with various polarizations. They have opened coherent X-ray diffraction method, X-ray free electron laser technology and high resolution soft X-ray spectroscopy, respectively.

B. Projects

Project name	Category	Started	Completed
Construction of Micro Protein Crystallography beamline	MEXT, Targeted Proteins Research Program	2007	2011
Development of X-ray diffraction microscope for the freeze biological samples	MEXT, XFEL reseach promotion program	2008	2010
SR Nano Beam Analysis	JST,ALCA	2010	2010

Center for Green/Nano-technology			

C. Members

as of March 1st, 2011

	number	Name
Research Scientist	1	Masaki Yamamoto
Technical Scientist	0	
Research Staff	4	Hironori Murakami, Kouichi Hashimoto, Eriko Nango, Tetsuya Haruna
Technical Staff	0	
Visiting Researchers	32	
Trainees	10	

D. Funding

(million yen)

	FY2008	FY2009	FY2010
Laboratory budget from RIKEN	34	28	12
Competitive fund in RIKEN	0	3	0
Competitive fund outside RIKEN	256	216	417
Other fund from University, Private foundations etc.	0.7	0	0

3-1-1. SR Life Science Instrumentation Unit / 生命系放射光利用システム開発ユニット

Unit Leader; Masaki Yamamoto, Ph D. / 山本 雅貴
Since November 2008

A. Research Topics (Highlights)

1. Research and developmet of instrumentations for structural biology beamlines

At SPring-8, protein crystallography beamlines have been constructed and developed to achieve the data collection for smaller crystals and more rapid structure analysis.

The new undulator beamline at SPring-8 for protein micro-crystallography, named RIKEN Targeted Proteins Beamline (BL32XU), had been constructed and user operation for "Targeted Proteins Research Program" started in May 2010. Recently, users' demands for high-quality data collection from protein micro-crystals have been increasing. To achieve protein micro-crystallography, data collection system with very high signal-to-noise ratio of diffraction spots from micro-crystals should be essential. Through the user operation of the beamline BL32XU, some precious experimental results have been obtained, especially for smaller and lower quality protein crystals. For example, the beamline provided high quality diffraction dataset by using a micro-sized crystal harvested from the initial crystallization condition. This result proved the beamline ability for achieving protein micro-crystallography both by increasing reflection intensities and by reducing background scattering from sample environments.

The SPring-8 standard automatic system to execute successive diffraction experiments with sample auto-changer SPACE and operation software BSS was developed at RIKEN Structural Genomics Beamlines (BL26B1 & BL26B2). The beamlines have been routinely operated with automatic system in last eight years, contributing to efficient data collection for a vast amount of samples for structural genomics research (Protein 3000 project). In order to achieve much more efficient and automated diffraction data collection, automatic crystal screening, real-time monitoring of radiation damage, automatic crystal centering and so on are under development. Furthermour, based on that automatic system, we have developed the remote access data collection system and started user operation at BL26B1 in 2010. The system provides users an interface on PCs at laboratory to operate crystal mounting and centering, diffraction measurement, data download and so on. The remote system works under the beamline interlock permissions, which has been developed as a common platform of SPring-8, to be able to install at all beamlines. The system is expected to be utilized in a complementary style, which enables distant users to conduct more flexible and real-time expeririments, compared to the mail-in data collection.

By the improvement of ab initio modeling from the protein solution by small angle X-ray scattering (SAXS), it has become widely used to predict the molecular shapes in the solution. Therefore the demand for the strucuture analysis of protein complex and the structure change analysis of proteins in the solution is increased. Structure Biology Beamline I (BL45XU) is operated for SAXS and small and wide angle X-ray scattering (SWAXS) measurements. To satisfy these demands, we are developing an automatic liquid handler for SAXS measurement. The system stores 96 protein solutions at constant temperature, and exchanges the solutions in the measurement cell in sequence. To install the system into the beamline, we will achieve the highthroughput measurement in SAXS. We are also exploring a SAXS measurement from high diluted protein solution and a fast time-resolved measurement for dynamical analysis of proteins in the solution. We installed a photon counting 2D detector, PILATUS 300K-W. The

detector is possible to detect a single photon without any background noise and to collect images at high frame rate up to 200 Hz. By development of the liquid handler and installation of new detector, we will promote biological SAXS for both the highthroughput measurement and the ultimate satate measurement.

2. Research and development of new techniques for structural biology experiments

To overcome the difficulties of protein crystallography utilizing high-brilliant X-ray beam, the research for optimizing the data collection strategies are essential. The strategies should be determined based on the modelling of statistical characteristics of the data such as diffracting power, crystal radiation damage, anomalous, and hardware limitation. The critical limit of absorbed dose for a better data collection was supposed to be around 10^6Gy. Diffracting power of a crystal can be modeled as 'B-factor' by evaluating a few diffraction images acquired with different amounts of photon flux. Estimated B-factor is used to predict the resolution limit with an arbitrary exposure time. By taking into account and balancing both of a lifetime and a diffracting power of a sample crystal, the best experimental condition can be determined. Based on the concept, we are developing a new application for suggesting the better data collection conditions through a beamline control softoware.

We have been evaluating the high-speed X-ray CMOS detector. The fundamental characteristics of the detector such as linearity, uniformity, and spatial resolution showed sufficient performance as the detector for protein crystallography. Making the best use of the high frame rate of the detector, we have been developing 'the high-speed diffraction based crystal alignment system'. Recently, sample visualization tends to be more difficult because targeted crystal size is getting to be smaller. In this case, it is preferreble to conduct positional scan in a cryo-loop at where a stronger diffraction appears on the X-ray detector. A readout time of the detector governs the total experimental time in this experiment. The X-ray CMOS detector enables this scan ten times as fast as X-ray CCD detector. We have been developing the automatic crystal alignment system based on this method.

It will be possible to collect diffraction data from a protein micro-crystal sized in the range from 1 to 10 μm in BL32XU. However, it is difficult to manipulate the protein micro-crystal by hands, because the protein micro-crystals are very small and fragile. We are also developing an automatic micro-crystal pick-up system applying optical tweezers to manipulate the fragile protein crystals.

In utilizing X-ray Free Electron Laser in biological science, the structural analyses of non-crystalline mm-sub mm biological particles are expected. Coherent X-ray diffraction microscopy (CXDM) has appeared as a new technique for the structure analysis of non-crystalline biological particle. Cryogenic X-ray coherent imaging system is developing by collaboration with Prof. Nakasako of Keio University. The samples are flash-frozen by liquid-ethane to reduce radiation damage. The system is composed of a high-precision goniometer, a liquid-He-cooled sample holder and a device to transfer frozen samples to the holder in the vacuum chamber. Preliminary coherent X-ray diffraction microscopy experiments at cryogenic temperature have been performed at BL29XUL. From the diffraction pattern of gold colloidal particles, the real space image was retrieved by an algorithm combining the hybrid-input-output and shrink-wrap method.

3. Operation of the RIKEN structural biology Beamlines

We support user experiments and beamline operations of four RIKEN structural biology beamlines: BL26B1, BL26B2, BL32XU and BL45XU. Structural Genomic Beamlines (BL26B1&BL26B2) have implemented the automatic operation with the sample changer SPACE and web-based sample database. With this system, the mail-in data collection accepting samples sent from distant users have been contiuously provided. Also we have started the remote access data collection at BL26B1 from outside SPring-8 by developing the remote access software.

B. Research Subjects

(1) Research and Development of instrumentations for structural biology beamlines
(2) Research and Development of new technologies for structural biology
(4) Operation of the RIKEN structural biology Beamlines

C. Projects

Project name	Category	Started	Completed
Development of the micro-crystal handling technique	RSC Project to meet society's needs	2009	2009

D. Members

as of March 1st, 2011

	number	Name
Research Scientist	3	Masaki Yamamoto, Takaaki Hikima, Atsushi Shimada
Technical Scientist	3	Go Ueno, Yoshiaki Kawano, Kunio Hirata
Research Staff	0	
Technical Staff	0	
Visiting Researchers	16	
Trainees	14	

E. Funding

(million yen)

	FY2008	FY2009	FY2010
Laboratory budget from RIKEN	-	1	3
Competitive fund in RIKEN	-	6	0
Competitive fund outside RIKEN	-	0	0
Other fund from University, Private foundations etc.	-	0	0

F. Research Output

	FY2008	FY2009	FY2010
International Publications	3	5	7
Publications in Japanese	0	3	7
Oral Presentations	16	27	31
Patent Applications	1	1	0

a. Papers

(1) Hasegawa K., Hirata K., Shimizu T., Shimizu N., Hikima T., Baba S., Kumasaka T., and Yamamoto M.: “Development of a shutterless continuous rotation method using an X-ray CMOS detector for protein crystallorgaphy", J. Appl. Cryst. 42, 1165--1175 (2009).
(2) Kumasaka T., Aritake K., Ago H., Irikura D., Tsurumura T., Yamamoto M., Miyano M.,

Urade Y., and Hayaishi O.: “Structural basis of the catalytic mechanism operating in open-closed conformers of lipocalin type prostaglandin D synthase", J. Biol. Chem. 284, No. 33, 22344--22352 (2009).

(3) Ueno T., Abe M., Hirata K., Abe S., Suzuki M., Shimizu N., Yamamoto M., Takata M., and Watanabe Y.: “Process of Accumulation of Metal Ions on the Interior Surface of apo-Ferritin: Crystal Structures of a Series of apo-Ferritins Containing Variable Quantities of Pd(II) Ions", J. Am. Chem. Soc. 131, 5094--5100 (2009).

(4) Abe S., Hirata K., Ueno T., Morino K., Shimizu N., Yamamoto M., Takata M., Yashima E., and Watanabe Y.: “Polymerization of Phenylacetylene by Rhodium Complexes within a Discrete Space of apo-Ferritin", J. Am. Chem. Soc. 131, 6958--6960 (2009).

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(6) Hirata K., Ueno G., Nisawa A., Kawano Y., Hikima T., Shimizu N., Kumasaka T., Yumoto H., Tanaka T., Takahashi S., Takeshita K., Ohashi H., Goto S., Kitamura H., and Yamamoto M.: “New Micro-beam Beamline at SPring-8, Targeting at Protein Microcrystallography", AIP Conf. Proc. 1234, 901--904 (2010).

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(11) Watanabe A., Hirata K., Hagiwara Y., Yutani Y., Sugishima M., Yamamoto M., Fukuyama K., and Wada K.: “Expression, purification and preliminary X-ray crystallographic analysis of cyanobacterial biliverdin reductase", Acta Cryst. F 67, 313--317 (2011).

b. Oral Presentations (* Invited presentation)

(1) Yamamoto M., Hirata K., Ueno G., Kawano Y., Hikima T., Shimizu N., Kumasaka T.,: “Protein Micro-Crystallography with a SPring-8 Micro-Beam Beamline ", MX Frontiers at the One Micron Scale, Brookhaven NY, USA, July (2009).*

(2) Hasegawa K., Hirata K., Shimizu N., Baba S., Kumasaka T., and Yamamoto M.:”Starting routine operation of an X-ray CMOS detector at a SPring-8 protein crystallography beamline", 2009 Meeting of the American Crystallographic Association (ACA 2009), Toronto, Canada, July (2009).

(3) Hikima T., Shimizu T., and Yamamoto M.: “Development of the protein microcrystal handling technique using a laser tweezers", 25th European Crystallographic Meeting (ECM25), Istanbul, Turkey, Aug. (2009).

(4) Ueno G., Hirata K., Nisawa A., Kawano Y., Shimizu N., Kumasaka T., Tanaka T., Takahashi S., Takeshita K., Ohashi H., Goto S., Kitamura H., and Yamamoto M.: ¥New

micro-beam beamline at Spring-8, targeting at protein micro-crystallography", 10th International conference on synchrotron radiation instrumentation (SRI09), Melbourne, Australia, Sept.-Oct. (2009).
(5) Hirata K., Ueno G., Nisawa A., Shimizu N., Kumasaka T., Kawano Y., Hikima T., Tanaka T., Takahashi S., Takeshita K., Yumoto H., Ohashi H., Goto S., Kitamura H., Ohata T., Furukawa Y., and Yamamoto M.: “A new beamline at SPring-8 dedicatedd to protein microcrystallography", Joint Conference of the Asian Crystallographic Association and Chinese Crystallography Society (AsCA'09), Beijing, China, Oct. (2009).
(6) Yamamoto M.: “Protein micro-crystallography with a new micro-beam beamline at SPring-8", 2nd Workshop on FEL Science: Emerging X-ray Applications in Biological Systems, Kenting, Taiwan, Dec. (2009).*
(7) Yamamoto M.: “The roles of High-Brilliant Synchrotron radiation in macromolecular crystallography", 2nd International Conference on Drug Discovery and Therapy, Dubai, UAE, Feb. (2010)*.
(8) Yamamoto M., Hirata K., Kawano Y., Hashimoto K., Hikima T., Ueno G., Shimizu N., and KumasakaT.: “Protein Micro-Crystallography at SPring-8", 3rd Workshop on FEL Science: Emerging X-ray Applications in Biological Systems-2, Sapporo Japan, Oct. (2010).*
(9) Yamamoto M.: “The SPring-8 high-brilliant beamlines for macromolecular crystallography", AsCA 2010: The 10th Conference of the Asian Crystallographic Association (Asian Crystallographic Association), Busan, Korea, Oct.-Nov. (2010).*

G. Future Plan

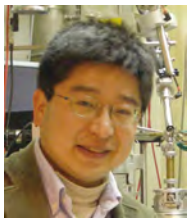
Life science research has dramatically progressed utilizing the high-brilliant X-ray source of synchrotron radiation facilities. At SPring-8, RIKEN beamlines have been developed and upgraded to achieve the data collection for smaller samples and more precise data acquisition, taking full advantage of the bright and coherent light source. New technology commonly required among these fields is the direct observation of structures and functions dynamically evolving in a given sample in more small scale (nano-meter) and/or short time domain.

In structural biology field, the construction of the protein micro-crystallography beamline (BL32XU) had been finished in 2010, when we started protein micro-crystallography experiments to solve the difficult protein structures. Although most ongoing structural biology researches of the unit are related to protein micro-crystallography, we are promoting R&Ds for micro-crystal handling and data collection strategies coupling with ‘Radiation Damage’ in accelerated manner. We will also continue the current activitie of ‘Beamline Automation’, since these investigations will accelerate wide varieties of structural biology research. Since the size of the protein crystals will continue to diminish, the imaging of a single molecule of proteins can be regarded as an ultimate extension in this direction. From viewpoint of the life science, there must be an R&D project conducted at SPring-8 and XFEL to visualize the biological hierarchy from cell-level to organ-level with a spatial resolution of nano-meter.

At RIKEN, a huge number of biology projects are present and a number of new projects will start more in near future. We will continue the R&Ds of new technologies not only for protein crystallography but also coherent imaging at SPring-8 beamlines and XFEL in future.

The other mission of the unit is the user support at the RIKEN beamlines. In order to make it easier for users to access beamlines, we will continue the user support, which will include education of new comers to SPring-8 and SR research from relating laboratories. The user support should be much more sufficient by increasing staffs and post-doctoral fellows.

H. Curriculum Vitae (Chief Scientist)



NAME: Masaki YAMAMOTO

DATE OF BIRTH: September 5,1963

EDUCATION:

1986: Graduated from Department of Bioengineering, School of Engineering Science, Osaka University,

1988: Master Degree from Department of Bioengineering, Graduate School of Engineering Science, Osaka University

1991: PhD degree from Department of Macromolecular Science, Graduate School of Science, Osaka University

DEGREES: PhD degree (Science, Osaka University)

APPOINTMENTS:

1991-1997: Research Scientist, Biophysics Laboratory at RIKEN

1997-2002: Research Scientist, Structural Biophysics Laboratory at Harima Institute of RIKEN

2002-2004: Senior Research Scientist, Coherent X-ray Optics Laboratory at Harima Institute of RIKEN

2002-2007: Joint Appointment of Group Leader, Structural Biology Group, Research & Utilization Division, JASRI

2004-2008: Team Leader, Synchrotron Radiation Instrumentation Team at Harima Institute of RIKEN

2005-: Joint Appointment of Visiting Professor, University of Hyogo

2005-2007: Joint Appointment of Deputy Director, Research & Utilization Division, JASRI

2008-: Group Director, Research Infrastructure Group at Advanced Photon Technology Division at at Harima Institute of RIKEN

2010-: Division Leader, Advanced Photon Technology Division at at Harima Institute of RIKEN

ACADEMIC ACTIVITIES:

2008-: Councilor, the Crystallography Society of Japan

2008-2009: Councilor, Japanese Society for Synchrotron Radiation Research

2007-2009: Secretary of Event, Japanese Society for Synchrotron Radiation Research

2003: Hyogo SPring-8 Award from the Hyogo Prefecture

2005: Research Award from the Crystallography Society of Japan

3-1-2. SR Materials Science Instrumentation Unit / 物質系放射光利用システム開発ユニット

Unit Leader; Yoshihito Tanaka, Dr. of Science / 田中　義人
Since January 1, 2009

A. Research Topics (Highlights)

1. Development and demonstration of advanced beamline technology for materials science
Advanced system of time- and space-resolved measurement has been developed for materials science research at RIKEN beamlines of SPring-8. We installed an X-ray fast mechanical chopper and timing monitoring system in BL19LXU, and have demonstrated picosecond time-resolved X-ray diffraction measurements for laser-induced lattice dynamics in semiconductor crystals. Nano-focusing mirror system has also been installed to achieve a 100 nm-sized X-ray beam for space-resolved X-ray magnetic scattering research. In BL44B2, a high resolution powder diffractometer has been developed for structural materials science.

2. Subpicosecond single shot coherent imaging using a free electron laser
Ultrafast coherent imaging utilizing free electron laser (FEL) with ultra-short pulse-width and full spatial coherence is a technique with the potential for new science. X-ray FEL ultimately enables the observation of atoms in motion in femtosecond time scale. We successfully demonstrated single shot coherent imaging using subpicosecond pulsed EUV-FEL from the SCSS test accelerator.

B. Research Subjects

(1) Development of advanced X-ray measurement methods using the SPring-8 beamlines
(2) Investigation for the measurement methods using next generation SR sources
(3) Sample monitoring system and quick switching system of users' SR experiments

C. Projects

Project name	Category	Started	Completed
Core Research for Evolutional Science and Technology	JST, CREST	2004	2009
XFEL research promotion program	MEXT, XFEL Research Promotion Program	2006	2010
Grant-in-Aid for Scientific Research (B)	MEXT, Grant-in-Aid for Scientific Research (B)	2009	2012

D. Members

as of March 1st, 2011

	number	Name
Research Scientist	2	Yoshihito Tanaka, Kenich Kato
Technical Scientist	0	
Research Staff	2	Atsushi Nisawa, Hiromi Sato, Kiminori Ito

Technical Staff	0	
Visiting Researchers	0	
Trainees	2	

E. Funding

(million yen)

	FY2008	FY2009	FY2010
Laboratory budget from RIKEN	-	1	2
Competitive fund in RIKEN	-	0	0
Competitive fund outside RIKEN	-	19	20
Other fund from University, Private foundations etc.	-	0	0

F. Research Output

	FY2008	FY2009	FY2010
International Publications	1	6	5
Publications in Japanese	0	3	3
Oral Presentations	4	13	15
Patent Applications	0	0	1

a. Papers

(1) Tanaka Y. ,Fukuyama Y. ,Yasuda N. ,Kim J. ,Murayama H. ,Kohara S. ,Osawa H. , Nakagawa T. ,Kimura S. ,Kato K. ,Yoshida F. ,Kamioka H. ,Moritomo Y. ,Matsunaga T. ,Kojima R. ,Yamada N. ,Toriumi K. ,Ohshima T. ,Tanaka H. ,and Takata M. : "Development of Picosecond Time-Resolved Microbeam X-ray Diffraction Technique for Investigation of Optical Recording Process", Jpn. J. Appl. Phys., 48, 03A001 (2009)

(2) Yasuda N. ,Murayama H. ,Fukuyama Y. ,Kim J. ,Kimura S. ,Toriumi K. ,Tanaka Y. ,Moritomo Y. ,Kuroiwa Y. ,Kato K. ,Tanaka H. ,and Takata M. : "X-ray diffractiometry for the structure determination of a submicrometre single powder grain", J. Synchrotron Rad., 16, 352--357 (2009)

(3) Moritomo Y., Nakagawa T., Fukuyama Y., Yasuda N., Osawa H., Kim J., Kamioka H., Kato K., Tanaka Y., Kimura S., Nakada F., Ohkoshi S., Tanaka H., Takata M.: "Photoinduced dynamics of prussian blue type cyanide", J.Phys.Conf.Ser.148, 012028 (2009)

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(7) Fukuyama Y. ,Yasuda N. ,Kamioka H. ,Kim J. ,Shibata T. ,Osawa H. ,Nakagawa T. ,Murayama H. ,Kato K. ,Tanaka Y. ,Kimura S. ,Ohshima T. ,Tanaka H. ,Takata M. ,and

Moritomo Y. : "Simultaneous measuerment of picosecond lattice and charge dynamics in Co-Fe cyanides", Appl. Phys. Express, 3, 016601 (2010)
(8) Tanaka Y. ,Ohshima T. ,Fukuyama Y. ,Yasuda N. ,Kim J. ,Osawa H. ,Kimura S. ,Togashi T. ,Hara T. ,Kamioka H. ,Moritomo Y. ,Tanaka H. ,Takata M. ,Sengoku H. , Nonoshita E. : "High-precision time delay control with continuous phase shifter for pump-probe experiments using synchrotron radiation", AIP Conference Proceedings, 1234, 951-954 (2010)
(9) Fukuyama Y. ,Yasuda N. ,Kimura S. ,Tanaka Y. ,Osawa H. ,Kim J. ,Murayama H. , Moritomo Y. ,Toriumi K. ,Tanaka H. ,and Takata M. : "Pump-probe X-ray Diffraction Technique for Irreversible Phase Change Materials", AIP Conference Proceedings, 1234, 215--218 (2010)
(10) Nishino Y. ,Tanaka Y. ,Okaya M. ,Uozaki Y. ,Nozaki K. ,Yabashi M. ,Nagasono M. , Matsui S. ,Ishikawa T. ,and Matsubara E. : "Femtosecond Snapshot Holography with Extended Reference Using Extreme Ultraviolet Free-Electron Laser", Appl. Phys. Express, 3, 10271 (2010)
(11) Hoshino T., Kikuchi M., Murakami D., Mitamura K., Harada Y., Ito K., Tanaka Y., Sasaki S., Takata M., Takahara A.:"X-ray photon correlation spectroscopy of silica particles grafted with polymer brush in polystyrene matrix", J. Phys. Conf. Ser., 272, 012020 (2011)
(12)Tanaka Y., Uozaki Y., Nozaki K., Ito K., Yamasaki K., Terauchi H., Takahashi I., Tahara K., Ishikawa T.:"Time-resolved X-ray diffraction studies of laser induced acoustic pulse generation in semiconductors using synchrotron radiation", J.Phys.Conf.Ser.,287,012018 (2011)
(13) Tanaka Y., and Adachi S.:"Detectors for timing monitor II (Streak cameras and fast photodetectors)", JSSRR, 22(2), 77-84 (2009)
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(15) Tanaka Y. : "Time-resolved X-ray diffraction studies of coherent lattice dynamics using synchrotron radiation", Journal of the Vacuum Society of Japan, 53(5), 327--335 (2010)
(16) Nishino Y., Tanaka Y. ,and Matsubara E.: "Toward ultrafast coherent imaging of materials sceicence phenomena with FEL", JSSRR, 23(5), 322-324 (2010)

b. Oral Presentations (* Invited presentation)

(1) Tanaka Y. : "Time-resolved x-ray studies using synchrotron radiation –For fs laser-induced structural change of materials–",_Workshop on POSTEC-RIKEN joint research program, SPring-8, Harima, Japan, Oct. (2009)*
(2) Tanaka Y. : "Time-resolved X-ray SR experiments using synchronized femtosecond pulsed laser ", Extreme Photoncs Seminar, Wako, Japan, June (2010)*
(3)Time-resolved X-ray diffraction studies of laser induced acoustic pulse generation in semiconductors using synchrotron radiation, Y. Tanaka, Y. Uozaki, K. Nozaki, K. Ito, K. Yamasaki, H. Terauchi, I. Takahashi, K. Tahara, T. Ishikawa, Laser-Ultrasonics 2010 (LU2010), Talence, France, 2010/7/5-8 (2010)
(4) Tanaka Y. : "Development of X-ray free electron lasers and future experiments", Symposium of Oyo Buturi, Nagasaki, Japan, Sep. (2010)*

G. Future Plan

The unit will contribute to development of new technology, which is useful for the future experiments using the brilliant SR X-ray beam and X-ray free electron laser (XFEL). Time- and space-resolved X-ray scattering method will be demonstrated for materials science in order to show how to use the coherent XFEL beam and the brilliant SR X-rays produced at the storage ring of SPring-8.

H. Curriculum Vitae (Unit Leader)

NAME: Yoshihito Tanaka

DATE OF BIRTH: May 21, 1964

EDUCATION:
1983-1987: The Univ. of Tokyo
1987-1989: Master course in The Univ. of Tokyo
1989-1991: Doctor course in The Univ. of Tokyo

ACADEMIC DEGREES: Dr.of Science (The Univ. of Tokyo; 1992)

APPOINTMENTS:
2009- : Unit Leader, SR Materials Instrumentation Unit
2006- : Joint Appointment of Senior Researcher, JASRI
2007- : Joint Appointment of Visiting Professor, Kwansei-Gakuin University
2010-2011: Joint Appointment of Visiting Professor, ISSP, The University of Tokyo

ACADEMIC ACTIVITIES:
2007-2010: Member of editorial board, Japanese Society for Synchrotron Radiation Research

3-1-3. Soft X-ray Spectroscopy Instrumentation Unit / 軟X線分光利用システム開発ユニット

Unit Leader; Masaki Oura, Dr. Sci. / 大浦 正樹
Since February 2010

A. Research Topics (Highlights)

1. Research and development of instrumentation for soft x-ray beamline BL17SU

The Soft X-ray Spectroscopy Instrumentation Unit is primarily in charge of the development, improvement and generalization of various spectroscopic tools as well as cutting-edge utilization technologies for soft x-ray (SX) spectroscopy, we are also responsible for providing the infrastructure to raise the user's convenience. For this purpose, an improvement of the quality of SX beam to be provided at the versatile space of the b-branch of BL17SU, where users can connect their own apparatuses as carry-in instruments, is planned to enhance the photon flux density at the sample position. In order to accomplish a small beam-spot-size on the sample at the versatile space, a set of refocusing mirrors with a Kirkpatrick-Baez configuration has been newly installed. By using this refocusing mirrors system, a focal size of less than a few tens of microns will be achieved, and then the photon flux density will be improved to be more than indeed 50,000 times or more. This versatile space will be operated as a carry-in station for users and the intense soft x-ray beam with small spot-size will be available early in fiscal 2011.

2. Research and development of new technique for soft x-ray spectroscopy

After starting of the Soft X-ray Spectroscopy Instrumentation Unit, the research and development for the time-resolved SX spectroscopy has been initiated. For the first step, a time-resolving two dimensional position sensitive detector (TR-PSD) was applied to the SX emission spectrometer. The existing flat-field spectrometer was modified for this purpose by replacing the CCD detector with the TR-PSD. The end-station equipped with the time-resolved SX emission spectrometer was installed on the b-branch of BL17SU.

For the data handling, two sets of signal processing system were developed. One is the data acquisition system based on the CAMAC, which can be widely and easily applicable to the variety of the experiments such as the X-ray Emission PhotoElectron Coincidence Spectroscopy (XEPECS). The other one is the newly introduced signal processing system purchased from German company, for which this work is supported by RIKEN SPring-8 Center Project of FY2009 to meet society's needs. The new signal processing system consists of a 8-channel front-end electronics (amplifier and constant fraction discriminator) and a 8-channel time-to-digital converter based on the CERN HPTDC. By using this new system combined with a high-speed PC, data acquisition rate at least 100 kHz to > 1 MHz (CPU dependent) will be available with high timing resolution (< 100ps, nominal least bit 25 ps), unlimited range and number of hits with dead-time of 5 ns. These signal processing system and the time-resolved SX emission spectrometer are almost ready for use to advance the time-resolved SX spectroscopy.

B. Research Subjects

(1) Development, improvement and generalization of cutting-edge utilization technologies for soft x-ray spectroscopy

(2) Research and development of SR beamline components
(3) Research and development of pump-probe soft x-ray spectroscopy using high brilliant soft x-ray radiation and femto-second laser

C. Projects

None

D. Members

as of March 1st, 2011

	number	Name
Research Scientist	1	Masaki Oura
Technical Scientist	0	
Research Staff	1	Tatsuya Wagai
Technical Staff	0	
Visiting Researchers	0	
Trainees	0	

E. Funding

(million yen)

	FY2008	FY2009	FY2010
Laboratory budget from RIKEN	—	—	2
Competitive fund in RIKEN	—	—	0
Competitive fund outside RIKEN	—	—	0
Other fund from University, Private foundations etc.	—	—	0

F. Research Output

	FY2008	FY2009	FY2010
International Publications	—	—	7
Publications in Japanese	—	—	0
Oral Presentations	—	—	28
Patent Applications	—	—	0

a. Papers

(1) Miyawaki J. , Chainani A. , Takata Y. , Mulazzi M. , Oura M. , Senba Y. , Ohashi H. , and Shin S. : “Out-of-Plane Nesting Driven Spin Spiral in Ultrathin Fe/Cu(001) Films”, Phys. Rev. Lett. **104**, 066407-1—066407-4 (2010)
(2) Tanaka Y. , Kojima T. , Takata Y. , Chainani A. , Lovesey S.W. , Knight K.S. , Takeuchi T. , Oura M. , Senba Y. , Ohashi H. , and Shin S. : “Determination of Structural Chirality of Berlinite and Quartz using Resonant X-ray Diffraction with Circularly Polarized X-rays”, Phys. Rev. B**81**, 144104-1—144104-9 (2010)
(3) Bhobe P.A. , Chainani A. , Taguchi M. , Takeuchi T. , Eguchi R. , Matsunami M. , Ishizaka K. , Takata Y. , Oura M. , Senba Y. , Ohashi H. , Nishino Y. , Yabashi M. , Tamasaku K. , Ishikawa T. , Takenaka K. , Takagi H. , and Shin S. : “Evidence for a Correlated Insulator to Antiferromagnetic Metal Transition in CrN”, Phys. Rev. Lett. **104**,

236404-1—236404-4 (2010)
(4) Oura M. : “Study of Inner-Shell Excitation and Relaxation Processes in Atomic and Ionic Neon by means of Soft X-ray Spectroscopy”, Plasma Sci. Technol. **12**, 353—360 (2010)
(5) Oura M. , Takahashi O. , Gejo T. , Tokushima T. , Horikawa Y. , Senba Y. , Ohashi H. , and Shin S. : “Vibrationally Resolved Resonant X-ray Emission Spectra of Diatomic Molecules”, J. Phys. Conf. Series **235**, 012016-1—012016-11 (2010)
(6) Nishizawa K. , Kurahashi N. , Sekiguchi K. , Mizuno T. , Ogi Y. , Horio T. , Oura M. , Kosugi N. , and Suzuki T. : “High-Resolution Soft X-ray Photoelectron Spectroscopy of Liquid Water”, Phys. Chem. Chem. Phys. **13**, 413—417 (2010)
(7) Ohtsuki T. , Chainani A. , Eguchi R. , Matsunami M. , Takata Y. , Taguchi M. , Nishino Y. , Tamasaku K. , Yabashi M. , Ishikawa T. , Oura M. , Senba Y. , Ohashi H. , and Shin S. : “Role of Ti 3d Carriers in Mediating the Ferromagnetism of Co:TiO_2 Anatase Thin Films”, Phys. Rev. Lett. **106**, 047602-1—047602-4 (2011)

b. Oral Presentations (* Invited presentation)

(1) Oura M. , Wagai T. , Tanaka Y. , Togashi T. , Senba Y. , Ohashi H. , and Shin S. : “A test for the time-resolved spectroscopy by means of soft x-ray emission spectroscopy II”, 24th Annual Meeting of Japanese Society for Synchrotron Radiation Research (JSR11), Tsukuba, Japan, Jan. (2011)

G. Future Plan

Our unit will contribute to the development, improvement and generalization of various spectroscopic tools as well as cutting-edge utilization technologies for SX spectroscopy to be performed at BL17SU. We will also keep making progress of the infrastructure of BL17SU to achieve higher performance of the beamline. We would like to continue to develop the time-resolved SX emission spectroscopy in order to advance the optical and materials science by using high brilliant SX undulator radiation from BL17SU. This time-resolved spectroscopic method will be applied to carry out a dynamic observation of the electronic states in transient phenomena stimulated by an external field, such as the electric field pulse, the magnetic field pulse and the femto-second laser pulse.

Furthermore, as a collaboration with the outside researchers, we would like to start a joint research on carbon nanotubes (CNTs) for device applications. CNTs are well known materials attracting great interest due to their unique physical, chemical, mechanical, and electronic properties. Various device applications of CNTs to field electron emitters have been investigated so far. For some device applications, it is found recently that the introduction of defects into CNTs is effective to control the characteristics of the device. For this purpose, we will employ the ion-beam irradiation method for introducing the defects into vertically aligned CNTs grown on substrate. An ion source of the photon-ion merged-beam apparatus installed at BL17SU will be used for the ion-beam irradiation onto the vertically aligned CNTs target, and the surface-modified target will be analyzed *in-situ* by the SX spectroscopy at BL17SU. The unique feature of our apparatus is the selectivity of the ionic species, the charge state as well as the kinetic energy for the ion-beam irradiation. The capability of *in-situ* analysis is also the unique feature. Such experiments can only be performed at BL17SU

H. Curriculum Vitae (Unit Leader)

NAME: Masaki OURA

DATE OF BIRTH: August 14, 1962

EDUCATION:

1986: Graduated from Faculty of Engineering, Hosei University
1988: Master Degree from Graduate School of Engineering, Hosei University
1991: Ph.D. from Graduate School of Science, Tohoku University

ACADEMIC DEGREES: Ph.D. (Science, Tohoku University)

APPOINTMENTS:

1991-1996 : Scientist, Atomic Physics Lab., RIKEN
1996-1998 : Scientist, SPring-8 Project Team, RIKEN
1998-1999 : Scientist, Coherent Synchrotron Light Source Lab., Harima Inst., RIKEN
1999-2007 : Scientist, Soft X-ray Spectroscopy Lab., Harima Inst., RIKEN
2003 Autumn : Visiting Professor, Fudan University, China
2007-2010 : Scientist, Coherent X-ray Optics Lab., RIKEN SPring-8 Center, RIKEN
the second half year of 2008 : Visiting Associate Professor, Institute for Solid State Physics, The University of Tokyo
2010-present : Unit Leader, Soft X-ray Spectroscopy Instrumentation Unit, RIKEN SPring-8 Center, RIKEN

ACADEMIC ACTIVITIES:

Member of an organizing committee of the 24th Annual Meeting of Japanese Society for Synchrotron Radiation Research (JSR11)
Member of Physical Society of Japan
Member of Japanese Society for Synchrotron Radiation Research

3-1-4. SR Imaging Instrumentation Unit /イメージング利用システム開発ユニット

Unit Leader; Yoshiki Kohmura, Dr. Science /香村芳樹
Since Apr 2010

A. Research Topics (Highlights)

1. Infrastructure development for x-ray imaging and for evaluation of XFEL instruments

Our Unit has contributed to stable operations of all the experiments carried out at BL29XU. The research activity on coherent x-ray diffraction microscopy experiment has been extended to biological specimens at liquid nitrogen temperature since early 2010. Our Unit has contributed to aligning three large vacuum chambers along the optical axis.

We made a huge effort to improve the temperature stability inside the experimental hutch (EH)s of BL29XU. Several panel heaters were hung close to the inner wall of the EH2 and EH3 whose power were feed-back controlled by measuring the temperature at the experimental apparatus. The temperature stability of 0.05 K, thus achieved, promoted the precise measurement of coherent x-ray diffraction microscopy combined with scanning method (ptychography method) where the positional drift of the sample relative to the aperture was a serious concern. We modified the scanning x-ray fluorescence microscope instrument. To reduce the background of iron fluorescence lines, some parts of the instruments was replaced by parts made of PEEK polymer. We have developed user friendly software for the scanning x-ray fluorescence microscope.

Our Unit has developed an fast x-ray shutter composed of a rotating tantalum cylinder with slits which would be reliable over a year operation. The conventional x-ray shutters using solenoids fail to work properly after much shorter operations on the order of weeks. Our x-ray shutter achieved an opening time interval of around 1 milli-second much shorter than the commercially available x-ray shutters.

2. Berry-Phase Effect of X-rays inside deformed crystals

As a part of our activity on R&D of original x-ray imaging techniqures, we worked on and discovered an enhanced translation of an x-ray beam nearly parallel to the diffracting planes, over 5 millimeter distances in a deformed silicon crystal. This effect occurs near the Bragg reflection condition and was theoretically predicted in 2006. It is caused by the Berry-phase effect in phase space. The result opened a new frontier of research in fundamental physics. Moreover, many interesting applications would be derived using the discovered effect. For these reasons, our paper reporting this discovery was published in Physical Review Letters in 2010 as a highlight paper.

We have been working on the fundamental studies and applications of the novel x-ray translation effect. As for the application purpose, we have tested the effect using a deformed diamond crystal. High throughput, several % of the peak intensity, was observed at the crystal edge after propagating 5 millimeter inside the diamond crystal. This result showed that an x-ray wave guide with reasonably high throughput will be realized where x-ray beam trajectory is controllable inside crystalline material.

B. Research Subjects

(1)R&D of common equipments for the users of x-ray imaging and hard x-ray photo-electron spectroscopy
(2)R&D of original x-ray imaging techniqures
(3)R&D of optical elements for beam diagnosis and the utilization research at x-ray free electron laser

C. Projects

Project name	Category	Started	Completed
Observation of anomalous shift of x-ray wave packet inside crystal nearby Bragg reflection condition and application of the effect to x-ray wave guide	MEXT, Grant-in-Aid for Scientific Research (B)	FY2009※	FY2013

※research was conducted in Coherent X-ray Laboratory in FY2009

D. Members

as of March 1st, 2011

	number	Name
Research Scientist	1	Yoshiki Kohmura
Technical Scientist	0	
Research Staff	1	Seigo Yamamoto
Technical Staff	0	
Visiting Researchers	0	
Trainees	0	

E. Funding

(million yen)

	FY2008	FY2009	FY2010
Laboratory budget from RIKEN	0	0	2
Competitive fund in RIKEN	0	0	0
Competitive fund outside RIKEN	0	6※	6
Other fund from University, Private foundations etc.	0	0	0

※research was conducted in Coherent X-ray Laboratory in FY2009

F. Research Output

	FY2008	FY2009	FY2010
International Publications	1	2	1
Publications in Japanese	1	0	0
Oral Presentations	1	1	2
Patent Applications	0	1	0

a. Papers

(1) Kohmura Y. , Sawada K. , and Ishikawa T. : "Berry-Phase Translation of X rays by a Deformed Crystal", Physical Review Letters 104, 244801-1--244801-4 (2010)
(2) Kohmura Y. , Sawada K. , Taguchi M. , Ishikawa T. , Ohigashi T., and Suzuki Y. : “Formation of x-ray vortex dipoles using a single diffraction pattern and direct phase measurement using interferometry”, Applied Physics Letters 94, 101112-1--101112-3 (2009)
(3) Yoneda Y. , Kohmura Y. , and Suzuki Y. : “X-ray Diffraction Topography of BaTiO3 at Phase Transition Temperature”, Japanese Journal of Applied Physics 48, 09KF01 (2009)
(4) Jiang H. , Johnson D. R. , Song C. , Amirbekian B. , Kohmura Y. , Nishino Y. , Takahashi Y. , Ishikawa T. , and Miao J. : “Nanoscale Imaging of Mineral Crystals inside Biological Composite Materials using X-ray Diffraction Microscopy” Physical Review Letters 100, 038103-1-- 038103-4 (2008).

b. Oral Presentations (* Invited presentation)

(1) Kohmura Y. : "Enhanced Translation Effect of X-ray Wavepacket inside silicon deformed crystal", The Photon Factory workshop, 2011, Tsukuba, Japan, Jan. (2011)*
(2) Kohmura Y. : "Application of Novel Translation Effect inside deformed crystal", The 3rd workshop on FEL science, 2010, Hokkaido, Japan, Oct. (2010)*

G. Future Plan

(1) Infrastructure development for x-ray imaging and for evaluation of XFEL instruments

Our Unit will continue to make progress of the infrastructure of BL29XU to achieve a higher performance. First of all, we plan to improve the temperature stability in the experimental hutches. Second, we plan to replace the x-ray total reflection mirrors in the transport channel to new ones with improved surface roughness, to make more efficient use of the coherent x-rays. Third, we are discussing to construct a new EH in future, used mainly for the biological and medical imaging studies. Thereby we will reduce the loss of beamtime during the replacement of the large experimental equipments in and out of the EHs. Finally, we plan to improve our new shutter system to make it faster, more reliable and more user-friendly.

(2) Berry-Phase Effect of X-rays inside deformed crystals

There are many targets for the research based on the Berry-phase translation of x-rays. We will describe three of them as follows. First, we plan further to understand the fundamental nature of the Berry phase. Second, we plan to develop useful optical components using the Berry-phase translation effect. For example, we plan to develop precise x-ray wave guides by controlling the inner strain of the crystal. We also plan to develop an extremely fast switch that responds to the crystal strain (deformation) within pico-second time scale. Finally, we plan to develop novel methodologies for observing the phonons (dynamics of atomic displacements) in the pico-second time domain and develop them in future XFEL science.

H. Curriculum Vitae (Unit Leader)

NAME: Yoshiki Kohmura

DATE OF BIRTH: June 24, 1966

EDUCATION:

1985-1989: The Univ. of Tokyo
1989-1991: Master course in The Univ. of Tokyo
1991-1994: Doctor course in The Univ. of Tokyo

ACADEMIC DEGREES: Dr. of Science (The Univ. of Tokyo;1994)

APPOINTMENTS:

2002-2010: Senior Research Scientist, Coherent X-ray Optics Laboratory at Harima Institute of RIKEN
2010- : Unit Leader, SR Imaging Instrumentation Unit

ACADEMIC ACTIVITIES:

Member of Physical Society of Japan
Member of Japan Society of Applied Physics
Member of Japanese Society for Synchrotron Radiation Research

3-2. Protein Crystallography Research Group / タンパク質結晶構造解析研究グループ

Group Director; Tetsuya Ishikawa, Dr. Eng. / 石川 哲也
Since April 2007

Deputy Group Director; Naoki Kunishima, Dr. Sci. / 国島 直樹
Since May 2008

A. Research Topics (Highlights)

1. Protein Tectonics Platform

The Protein Tectonics Platform (PTP) at the RIKEN SPring-8 Center (RSC) enables beamline users to conduct efficient and complete protein science experiments within the SPring-8 campus. The PTP acts as an integrated hub by taking advantage of its location, just 5 minutes from the SPring-8 beamlines. The PTP's technical staff gained experience managing the state-of-the-art platform for protein crystallography with the national structural genomics project of Japan's "Protein 3000" initiative (FY 2002-2006). The high-performance facility provides for all aspects of crystal structure determination of proteins: gene manipulation and expression, purification, characterization, crystallization, in-house diffraction experiments, and crystallographic computations (Sugahara *et al.*, 2008, *J. Struct. Funct. Genomics*). The combination of the SPring-8 beamlines, the high-performance facility, and the experienced technical staff will promote innovative bio-science in the SPring-8 campus. Recently, the PTP was upgraded by adding a cell cultivation room for higher-order organism cells and a nano-dispensing crystallization apparatus to minimize the amount of protein sample.

In order to disseminate Protein 3000 results for the benefit of society, the PTP is now available to various research groups inside and outside RIKEN. The PTP provides users with a comprehensive protein study platform in a properly-maintained state. First, it was made available to all RSC scientists in June 2008, to facilitate the Center's various research activities. RSC scientists performed 927 experiments using the PTP in FY 2009. In addition, since June 2010, our group has sent experienced technical staffs of PTP to other RSC laboratories to support their research. Recently, a research paper supported by this temporary staff system was published (Ihara *et al.*, 2011, *Anal. Biochem.* **412**, 217-223). Second, the PTP has been available to Taiwanese scientists on a fee-paying basis since April 2009, based on a three-year contract with the National Synchrotron Radiation Research Center (NSRRC) of Taiwan. By March 2010, a total of 23 Taiwanese scientists visited our group to use the PTP, including initial trial use in 2008. Taiwanese scientists performed 193 experiments using the PTP in FY 2009. An international workshop for PTP users has been held at three cities in Taiwan (Taipei, Hsinchu, and Tainan) every year since September 2009. Third, as a contribution to the Collaborative Research Program with Industry funded by the Center for Intellectual Property Strategies of RIKEN, our group has accommodated a visiting scientist from a Japanese private company since October 2009, to perform collaborative research on the utilization of the PTP for structure-based drug design. To date, we successfully solved a few complex structures of target proteins with drug candidate compounds.

2. Integrated Database Project

At the RSC, a large-scale crystallographic analysis of bacterial proteins was performed as a contribution to the Protein 3000 Project, using SPring-8 X-rays in combination with a

high-throughput platform for structural studies. To benefit researchers in a broad range of life science fields, the experimental data from Protein 3000 have been compiled and published as a contribution to the Integrated Database Project funded by the MEXT ministry of Japan (FY 2007-2010). The RIKEN Bioinformatics and Systems Engineering Division (BASE) developed a database publication platform "Scientists' Networking System (RIKEN SciNeS; http://scines.org)" by which we performed the integrated database project. Database integration using RIKEN SciNeS uses the semantic web format that is suitable for data reuse and automatic processing, thereby allowing batch download of full data and reconstruction of data to make new databases. The RSC protein crystallography database was released from RIKEN SciNeS in July 2009 (Press release, 23 Jul. 2009).

Contents of the database are: 1) experimental data from nine species of bacteria that covers a large variety of protein molecules in terms of both evolution and properties (http://scines.org/item/rib220i); 2) experimental data of mutant proteins that were designed systematically to study the influence of mutations to the diffraction quality of protein crystals (http://scines.org/item/rib220i); and 3) experimental data of heavy-atom labeled proteins from which the user interface *Hatodas* (http://hatodas.harima.riken.jp) suggests potential compounds suitable for the preparation of heavy-atom derivatized protein crystals (http://scines.org/item/rib108i). Potential applications of the RSC database are as follows. The bacteria data 1) will provide reference information for the structural study of homologous proteins. To enhance the use for general researchers in biosciences, we released a comprehensible user interface *Bacpedia* (http://bacpedia.harima.riken.jp) in July 2010. The mutant data 2) have favorable characteristics for detailed structural comparisons between the mutant proteins because they share the same crystallization condition. This allows software development of high-precision homology modeling, for instance. The heavy atom data 3) may be applied to the in-situ imaging of bio-molecules with a heavy-atom labeling.

B. Research Subjects

(1) Application of Protein 3000 results for the benefit of society
(2) Development of advanced technologies for structural biology
(3) Structural study of proteins for industrial applications

C. Projects

Project name	Category	Started	Completed
Development of liquid/molecular beam generator for protein single particle analysis	MEXT, XFEL Research Promotion Program	2007	2010
Plant omics information and protein structure information	MEXT, Integrated Database Project	2007	2010
Role of electrostatic interactions in thermo-stabilization of proteins from hyperthermophile	MEXT, Grant-in-Aid for Scientific Research (C)	2008	2010
Development of bio-functional material toward recycling pollutant/rare metals	Hyogo STA	2010	2010
Development of novel	Institute Program	2010	2011

technologies for protein crystallization to upgrade crystal production system in SPring-8			
Thermodynamics of protein denaturation at high temperatures over 100 °C	MEXT, Grant-in-Aid for Scientific Research (C)	2010	2012
Investigation of acetyl-CoA carboxylase activation mechanism toward drug development	MEXT, Grant-in-Aid for Scientific Research (C)	2010	2012
Establishment of versatile protein crystallization method using zeolite as a crystallization substrate material	MEXT, Grant-in-Aid for Young Scientists (B)	2010	2012

D. Members

as of March 1st, 2011

	number	Name
Research Scientist	7	Tetsuya Ishikawa*, Naoki Kunishima, Hisashi Naitow*, Katsuhide Yutani, Michihiro Sugahara, Saori Maki (Yonekura), Padavattan Sivaraman
Technical Scientist	0	
Research Staff	2	Tomoyuki Tanaka, Yoshinori Matsuura,
Technical Staff	0	
Visiting Researchers	2	
Trainees	1	

* concurrently appointed

E. Funding

(million yen)

	FY2008	FY2009	FY2010
Laboratory budget from RIKEN	0	0	9
Competitive fund in RIKEN	5	30	3
Competitive fund outside RIKEN	15	17	14
Other fund from University, Private foundations etc.	0	21	19

F. Research Output

	FY2008	FY2009	FY2010
International Publications	12	12	10
Publications in Japanese	3	1	1

Oral Presentations	20	26	23
Patent Applications	0	0	0

a. Papers

(1) Sugahara M., Kageyama Y., and Kunishima N.: "A hands-free capillary system for protein crystallography from crystallization to data collection", J. Appl. Cryst. 42, 129-133 (2009)
(2) Sugahara M., Asada Y., Shimada H., Taka H., and Kunishima N.: "HATODAS II: heavy-atom database system with potentiality scoring", J. Appl. Cryst. 42, 540-544 (2009)
(3) Tanaka T., Shinkai A., Bessho Y., Kumarevel T., and Yokoyama S.: "Crystal structure of the manganese transport regulatory protein from *Escherichia coli*", Proteins 77, 747-751 (2009)
(4) Sugahara M., Shimizu K., Asada Y., Fukunishi H., Kodera H., Fujii T., Osada E., Kasazaki T., Sawada T., Chikusa H., Kondo K., Yorihiro A., and Kunishima N.: "Autolabo: an automated system for ligand-soaking experiments with protein crystals", J. Appl. Cryst. 43, 940-944 (2010)
(5) Asada Y., Kuroishi C., Ukita Y., Sumii R., Endo S., Matsunaga T., Hara A., and Kunishima N.: "Dimeric crystal structure of rabbit L-gulonate 3-dehydrogenase/λ-crystallin: insights into the catalytic mechanism", J. Mol. Biol. 401, 906-920 (2010)
(6) Matsuura Y., Ota M., Tanaka T., Takehira M., Ogasahara K., Bagautdinov B., Kunishima N., and Yutani K.: "Remarkable improvement in the heat stability of CutA1 from *Escherichia coli* by rational protein design", J. Biochem. 148, 449-458 (2010)
(7) Sugahara M., Kageyama-Morikawa Y., and Kunishima N.: "Packing space expansion of protein crystallization screening with synthetic zeolite as a heteroepitaxic nucleant", Crystal Growth & Design 11, 110-120 (2011)

b. Oral Presentations (* Invited presentation)

(1) Kunishima N.: "Perspective of technological development in protein structure determination: XFEL and X-ray crystallography", The 1st Workshop on FEL Science "Coherent Intense X-rays in Physics and Biology", Jeju, Korea, Feb. (2009)*
(2) Matsuura Y., Ota M., Takehira M., Bagautdinov B., Kunishima N., and Yutani K.: "Remarkable improvement of the heat stability of CutA1 from *E. coli* by protein engineering", The 8th European Symposium of the Protein Society, Zurich, Switzerland, Jun. (2009)
(3) Naitow H., Asada Y., and Kunishima, N.: "Introduction to PTP and RIKEN database for protein research", PTP User's Meeting at Hsinchu, Taipei and Tainan, Taiwan, Sep. (2009)*
(4) Kunishima N.: "Protein Tectonics Platform at RSC", Workshop on POSTECH-RIKEN Joint Research Program, SPring-8, Japan, Oct. (2009)*
(5) Kunishima N.: "Comprehensive platform for structural study of bio-molecules at RSC: XFEL and X-ray crystallography", The 2nd Workshop on FEL Science "Emerging X-ray Applications in Biological Systems", Kenting, Taiwan, Dec. (2009)*
(6) Sugahara M., Kageyama-Morikawa Y., and Kunishima N.: "Effective protein crystallization screening with synthetic zeolite Molecular Sieves as hetero-epitaxic nucleant", The Biophysical Society 54th Annual Meeting, San Francisco, California, USA, Feb. (2010)

(7) Kunishima N.: “Potential protein samples for diffractive imaging experiments using XFEL”, The 3rd Workshop on FEL Science “Emerging X-ray Applications in Biological Systems-II”, Hokkaido, Japan, Oct. (2010)*
(8) Naitow H. and Kunishima N.: “RIKEN SPring-8 Center Protein Tectonics Platform”, PTP User’s Meeting at Hsinchu, Taipei and Tainan, Taiwan, Nov. (2010)*
(9) Sugahara M.: “Protein crystallization screening with microporous synthetic zeolites Molecular Sieves”, Workshop on Structural Biology in Southern Taiwan with RIKEN PTP, Tainan, Taiwan, Feb. (2011)*

G. Future Plan

Because SPring-8 is the largest synchrotron radiation (SR) facility in the world, its efficient use in the world community is necessary to justify its huge operation/development costs. To meet this demand, we have to reconsider the current operational style of SPring-8 that tends to be biased toward beamline management, and we have to promote the construction of collaborative centers for applied SR research. One of such effort is the RIKEN RSC-Rigaku Collaboration Center since December 2010 to which our group provides effective protocols for protein research. In the future, we hope to establish other collaborative centers in the SPring-8 campus, which will provide various SR users outside RIKEN with all aspects of structural analysis from sample preparation to various applications including structure-based drug development.

To date, we have established the high-performance protein crystallography pipeline through a large-scale structure determination in the national structural genomics project “Protein 3000”. The experimental data from Protein 3000 were compiled and published as a contribution to the Integrated Database Project funded by the MEXT ministry of Japan. After the completion of these projects, facilities and databases are rearranged to establish the “Protein Tectonics Platform (PTP)” for protein studies at SPring-8, and opened to general bio-science researchers both inside and outside RIKEN. The PTP would provide a suitable platform for the collaborative centers in the SPring-8 campus.

We also study advanced technologies for difficult target proteins, including protein crystal engineering and the X-ray free electron laser (XFEL). These advanced technologies will be enhanced further to assist the structural determination of recalcitrant target proteins such as membrane proteins and supramolecular complexes. Based on the PTP with advanced technologies, we are now conducting collaborative research with a Japanese private company on the pharmaceutical application of protein structures, which may develop in the future to make another collaborative center.

In terms of international communications with SPring-8, Taiwan is the most advanced in Asia, because Taiwan has a dedicated beamline at SPring-8, has its own SR facility in the Taiwan island, and has a future plan for the construction of another larger SR facility. Since FY 2009, we have made available the PTP facility to Taiwan researchers on a fee-paying basis. Based on RIKEN-Taiwan communications to date, we recognize that Taiwan users have many good targets for structural studies including drug development and they hope international collaboration with us to resolve difficulties in structural determination. This RIKEN-Taiwan collaboration will be developed further considering the training of future generations, to serve as a model case of the efficient use of SPring-8 in Asia.

H. Curriculum Vitae (Group Director and Deputy Group Director)

Group Director

NAME: Tetsuya Ishikawa

Please refer to **Coherent X-Ray Optics Laboratory / 石川X線干渉光学研究室** (p.29)

Deputy Group Director

NAME: Naoki Kunishima

DATE OF BIRTH: 1 January, 1967

EDUCATION:

1989: B. Sc. In Biochemistry, Faculty of Science, Kanazawa University

1994: Ph. D., Department of Biochemistry, Graduate School of Science, Osaka University (Supervisor: Prof. Hiroshi Matsubara)

ACADEMIC DEGREES: Dr. Sci.

APPOINTMENTS:

1994-2001: Research Scientist, Department of Structural Biology, Biomolecular Engineering Research Institute

2001-2007: Team Leader, Highthroughput Factory (Advanced Protein Crystallography Research Group, Since Oct. 2004), RIKEN Harima Institute

2007-2008: Senior Scientist, Protein Crystallography Research Group

2008: Deputy Group Director, Protein Crystallography Research Group

2010: Team Leader, Protein Analysis System Development Team, RSC-Rigaku Collaboration Center (concurrently appointed)

ACADEMIC ACTIVITIES: None

4. New Beamline Construction

During the current period (2008-2011), the RSC has been working on construction of two new beamlines: one dedicated to Protein Micro-Crystallography and one for high-resolution Inelastic X-ray Scattering (IXS). These beamlines will expand the technical capabilities of SPring-8 to use highly-brilliant synchrotron radiation in order to explore new scientific fields.

4-1. BL32XU: RIKEN Targeted Proteins

Most proteins that are important to biological research are difficult to crystallize. Structural determination of biologically important proteins is often complicated by the small size of harvested single crystals. The collection of proper diffraction data from micro-crystals requires an innovative instrument to be designed. At the SPring-8, the RSC has completed construction of RIKEN's new undulator beamline dedicated for protein micro-crystallography, the Targeted Proteins Beamline (BL32XU). The beamline became available for user operations in May 2010.

The new beamline is designed to provide a brilliant X-ray micro-beam to collect high-quality data from micro-crystals. A target beam size of 1 μm was expected to provide data with a good signal-to-noise (S/N) ratio by reducing background scattering. The beamline layout is shown in Figure 1. The light source of the beamline is a 4.5 m hybrid in-vacuum undulator with a period of 2.6 cm (173 periods in total). A liquid-nitrogen cooled, double crystal Si(111) monochromator covers the required energy range of 8 - 20 keV. This high precision mechanism has been specially modified, with a design based on the SPring-8 standard monochromator. An aperture ("TC Slit" in Figure 1) in the monochromatic beam creates a virtual source. The beam from the virtual source is then focused onto the sample using elliptical K-B mirrors with a large reduction ratio of about 26 in the vertical, and 40 in the horizontal. The focusing mirror surfaces are fabricated with atomic-scale accuracy by Elastic Emission Machining (EEM) .

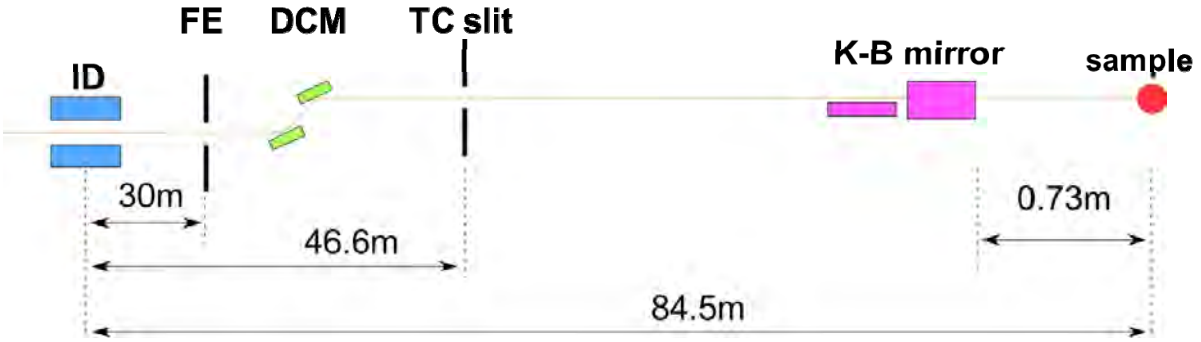


Figure 1. Schematic view of BL32XU. In this figure, the labels ID, FE, DCM, TC slit and K-B mirror represent the undulator, the front-end, the double crystal monochromator, the transport channel slit and the Kirkpatrick-Baez focusing mirrors, respectively.

The first beam was observed on October 3, 2009, and beamline commissioning was completed at the end of November 2009. The minimum beam size available is 0.9×0.9 μm^2 with a photon flux of 6×10^{10} photons/sec. (see Figure 2).
Research and development for low-background sample environments is now in progress. The first result produced a diffraction image with 2 Å resolution collected from a 2 x 2 x 2 μm^3 crystal. The RIKEN Targeted Proteins Beamline is expected to significantly benefit users by making optimal use of high quality diffraction data with a highly brilliant micro X-ray beam.

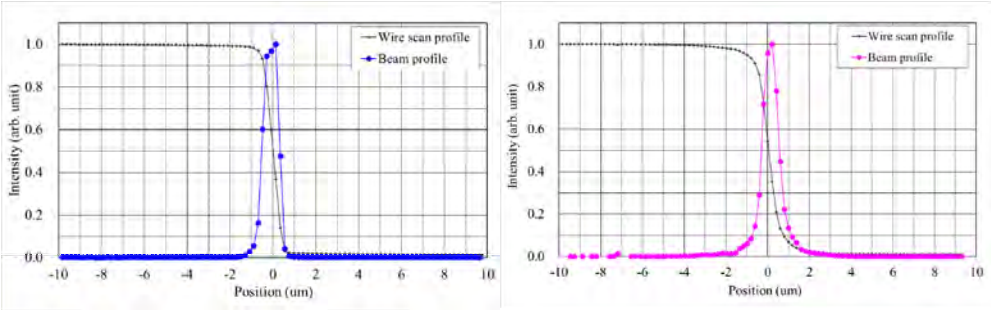


Figure 2. Focused beam profile at the sample position. The left and the right figures show the horizontal and the vertical beam profiles with a wire scan. In both directions, FWHM of the focused beam corresponds to 0.9 μm.

4-2. BL43LXU: RIKEN Quantum NanoDynamics

The RIKEN Quantum NanoDynamics (RQD) Beamline, BL43LXU, is a new beamline that takes advantage of SPring-8's capabilities to provide a uniquely powerful facility to investigate atomic-scale correlations in atomic and electronic dynamics using non-resonant inelastic x-ray scattering [1]. In particular, using the high, 8 GeV, electron energy at SPring-8, and in-vacuum insertion device (ID) technology, it is possible to make a small, 6mm, magnetic gap insertion device that is tunable in the fundamental from 14 to 26 keV. Use of a 30m straight section then allows a 15 m long ID, in three sections, to provide unprecedented flux in this energy range, > $6x10^{15}$ in conventional units (see Figure 1). Given the flux-limited nature of high-resolution IXS measurements, this is a significant and important improvement for world-wide IXS capability. Construction is now in progress and first light is expected before the end of 2011.

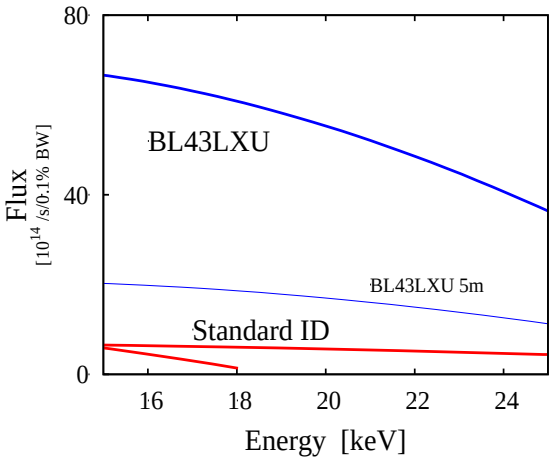


Figure 1. Performance of BL43LXU compared to a standard (32 mm period) insertion device as calculated using SPECTRA. The thin blue lines represent performance with only 1/3 of the installed ID.

The beamline layout is shown in Figure 2. A large spectrometer has a 10m arm for high resolution studies, providing energy resolution from <1 to ~40 meV and momentum resolution < $1nm^{-1}$. This arm will have a large, 42-element, analyzer array to allow parallel measurements of many momentum transfers simultaneously. A smaller, medium-resolution, spectrometer will relax both the energy resolution, 10 to 100 meV, and the momentum resolution, <5 nm^{-1}, to allow high-flux operation aimed at investigating electronic excitations. This spectrometer will use a new "temperature compensation" analyzer concept that is now under development [2].

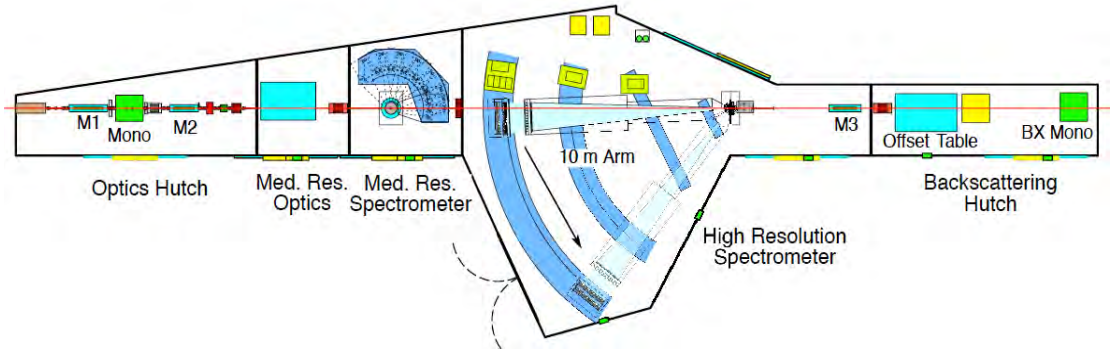


Figure 2: Hutch Layout for BL43LXU. The beam from the undulator is incident from the left, and for the high resolution spectrometer, is backscattered by the BX mono (far right), and impinges on the sample from the right. M1 is the nitrogen-cooled mirror, M2 is the mirror to return the beam to the horizontal and M3 is the focusing cylindrical mirror for high-resolution scattering. The length of the displayed hutches is 47m.

The power load of the x-ray beam from the insertion device is an important issue. While operating the ID in the fundamental gives the highest flux per unit of power in the central cone, the 15 m ID still will have a central cone with nearly 2 kW of power at the minimum ID gap. This is significantly beyond what is generally acceptable for applying power onto a silicon monochromator crystal, even when the crystal is cooled to liquid nitrogen temperatures. Thus the first optical element at the new beamline will be a grazing-incidence liquid nitrogen-cooled mirror, M1 in the figure. This configuration will reject higher harmonics and reduce power onto the monochromator to < 500W, while calculations suggest the thermal distortion of the mirror should remain < 0.4 μrad. A second mirror, M2, placed after the mono, will return the beam to the horizontal. The final beam spots at the spectrometers will be achieved using bent cylindrical mirrors, designed to have >90% throughput, with focal spot sizes expected to initially be about 25 microns in diameter at the high resolution spectrometer and 50 microns at the medium resolution spectrometer.

The present status of the beamline is that the hutches have been installed in the experimental hall, and many components have already been delivered. The necessary electron beam lattice changes to accommodate the small gap insertion devices are now in progress (since March 2011), and most of the high-heat-load front-end components have been installed. Most of the remaining components will be delivered by the end of May 2011, with installation and alignment in the hutches planned for the end of July. The first part (5m) of the insertion device will be installed in the summer of 2011, as will the large spectrometer. First light and the start of beamline commissioning are expected in October 2011. At this time, we are still waiting on budget approval to complete the remaining two 5m segments of the ID, though the cooling system to accept the power of the full 15m ID will be in place by the summer of 2011.

[1] More details may be found at http://user.spring8.or.jp/sp8info/?p=3138
[2] D. Ishikawa and A. Baron, Journal of Synchrotron Radiation 17, (2010) 12.

APPENDIX Ⅰ
The RIKEN Harima Institute

1. History of the RIKEN Harima Institute and the RIKEN SPring-8 Center

1-1. Development

In 1997, after six years of construction, RIKEN, in cooperation with the Japan Atomic Energy Research Institute (JAERI), completed SPring-8 (the Super Photon ring-8GeV). Located in west Harima, Hyogo Prefecture, SPring-8 is the world's largest synchrotron radiation facility. Since its opening, the management of operations and maintenance for SPring-8 has been entrusted to the Japan Synchrotron Radiation Research Institute (JASRI). RIKEN has been responsible principally for designing and constructing public-use beamlines as well as its own and other beamline-related facilities.

Upon opening SPring-8 for public use in October 1997, RIKEN established the RIKEN Harima Institute on-site at SPring-8. The RIKEN Harima Institute was initially conceived to promote the world's most advanced Synchrotron Radiation (SR) related research with the currently existing RIKEN Institute Laboratories (ILs). The RIKEN Harima Institute continued to launch additional ILs and in 1999 launched its first research initiative, the Synchrotron Radiation Research Network. Another project, the Protein 3000 at the High-throughput Factory; now called the Advanced Protein Crystallography Research Group at the Protein Tectonics Platform (PTP); was initiated in 2001 to use SPring-8 to analyze the basic structures and functions of major proteins.

At the end of September 2005, JAERI withdrew from the management of SPring-8 and RIKEN began oversight of the SPring-8 facility in collaboration with JASRI. RIKEN immediately set up the RIKEN SPring-8 Center (RSC) and its advisory council, the RIKEN SPring-8 Center Advisory Council (RSAC), under the RIKEN Harima Institute to fulfill its broader responsibility in developing the SPring-8 functions as its only entrustor.

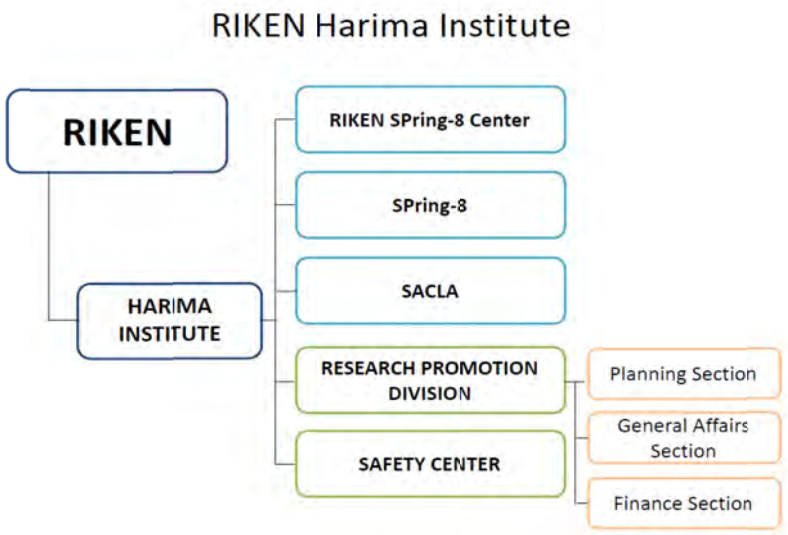
The X-ray Free Electron Laser (XFEL) of the national project started with a five-year-plan beginning in 2006. It was completed on schedule in March 2010, when the first synchrotron radiation was emitted (Refer to Section 4. The XFEL Project, for more details). The first lasing was achieved in June 2011.

In 2008, the RSC clarified its mission by reorganizing into three divisions: the Innovative Light Sources Division, the Photon Science Research Division, and the Advanced Photon Technology Division. The RSAC held in February 2009 provided an evaluation on the restructuring. As a result, the RSC appointed directors for each of the three divisions. Further, the RSC strengthened the existing positions by creating two Deputy Directors in both the Planning and Personnel sections and by establishing the RIKEN RSC-Rigaku Collaboration Center in December 2010. The RSC also set up the XFEL Research and Development Division in April 2011 after the XFEL Project ended.

Oct 1988 (Showa 63)		RIKEN and the Japan Atomic Energy Research Institute (JAERI) formed a joint project team to oversee construction of SPring-8 (Super Photon ring-8GeV), a large-scale synchrotron radiation facility
Jun 1989 (Heisei 1)		The Harima Science Garden City in West Harima, Hyogo Prefecture was officially chosen as the site of SPring-8
Dec 1990 (H 2)		The Japan Synchrotron Radiation Research Institute (JASRI) was established as a private foundation
Nov 1991 (H 3)		The construction of SPring-8 began
Oct 1994 (H 6)		The law regarding the promotion of public use of the Synchrotron Radiation Facility went into effect and JASRI was designated for its dedication
Mar 1997 (H 9)		The first synchrotron radiation was observed
Oct 1997 (H 9)		SPring-8 started operations for public use, and RIKEN established the RIKEN Harima Institute at the site of SPring-8
May 1999 (H 11)		The Synchrotron Radiation Research Network was launched
Apr 2001 (H 13)		High-throughput Factory (now known as the Protein Tectonics Platform (PTP)) was established
Oct 2003 (H 15)	First Midterm as IAI	RIKEN was reorganized as the Independent Administrative Institution (IAI) and the first 'Midterm' started (completed in 2008.03)
Nov 2004 (H 16)		The XFEL Research and Development Group was established
Sep 2005 (H 17)		JAERI withdrew from SPring-8 management
Oct 2005 (H 17)		The RIKEN SPring-8 Center (RSC) and its Advisory Council (RSAC) were established
Feb 2006 (H 18)		**RSAC 2006**
Mar 2006 (H 18)		The RIKEN XFEL Project Head Office was launched
Apr 2006 (H 18)		RIKEN and JASRI established the SPring-8 Joint Project for XFEL
Jul 2006 (H 18)		The applicable law was amended to promote "public use of Advanced Large Research Facilities"
Apr 2008 (H 20)	Second Midterm	The RSC was restructured with three divisions
Feb 2009 (H 21)		**RSAC 2009**
Apr 2010 (H 22)		Two Deputy Director positions were created at the RSC (in both the Planning and Personnel sections)
Dec 2010 (H 22)		The RIKEN RSC-Rigaku Collaboration Center was established
Mar 2011 (H 23)		The XFEL completed The RIKEN XFEL Project Head Office and SPring-8 Joint Project for XFEL ended
Apr 2011 (H 23)		The XFEL Research and Development Division was created in the RSC
Jul 2011 (H 23)		**RSAC 2011**

1-2. Organization

The relationship between the RIKEN Harima Institute and the RIKEN Spring-8 Center is described below. The Administrative Office division consists of the Research Promotion Division (including the Planning, Finance, and General Affairs Sections) and the Safety Center as a part of the RIKEN Harima Institute.



The number of employees in the Harima Research Promotion Division (Planning, Finance, and General Affairs Sections) and the Safety Center employees are as follows:

Permanent Staff	Fixed-term Contract Staff	Temporary Staff	Part-timers
14	15	4	10

1-3. Related Organizations

JASRI, nominated by RIKEN to be responsible for running SPring-8, was officially designated in 2006 as a "registered organization" by a law stipulating "the promotion of public use of advanced large research facilities". JASRI has undertaken the following missions mandated by that law:

1. to select research proposals for SPring-8 public use, and
2. to support and train users with the world's most advanced SR resources.

RIKEN entrusted JASRI as an organization selected by a public tender with the following missions:

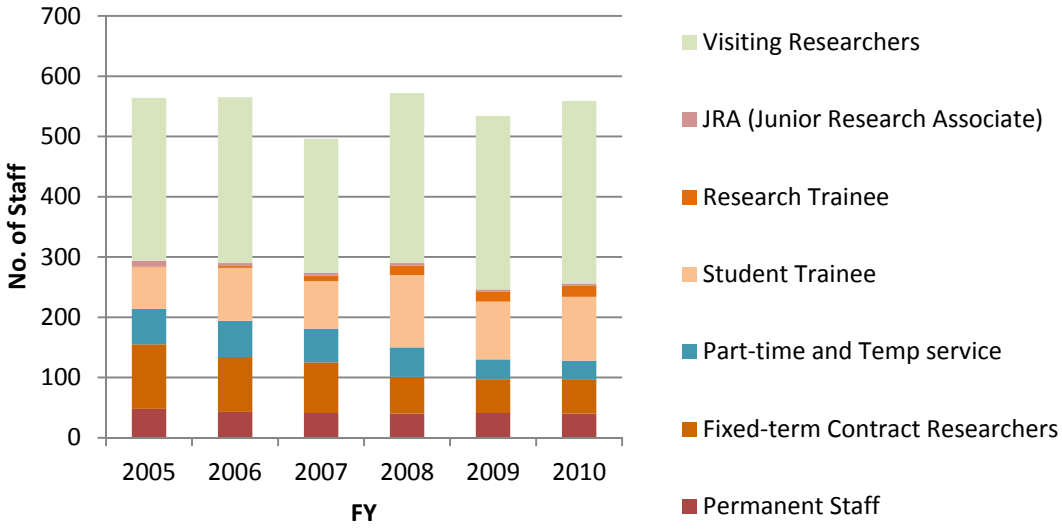
1. to operate, manage, maintain, and improve the accelerators and beamlines for public use (including R&D for experimental stations), and
2. to promote full use of the SPring-8 facility through expanding access to users from other fields such as industry and environmental science.

2. Trends of the RIKEN SPring-8 Center

Fiscal statistics relating to the RSC activities are presented in this section. The period of the XFEL project is from FY 2006 to 2010.

2-1. Human Resources

2-1-1. Number of Staff

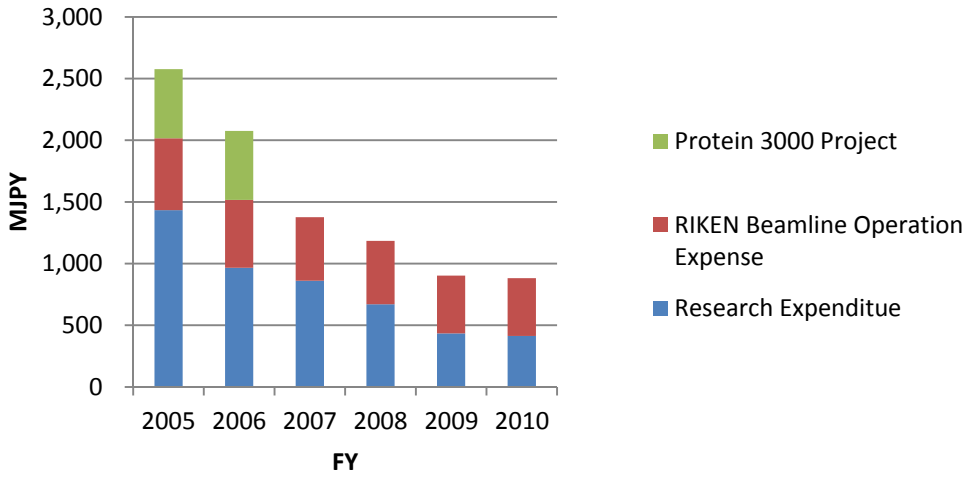


2-1-2. Proportions of Female and Foreign Researchers (Full-time Researchers)

Female	16.0%
Foreigners	7.4%

2-2. Income Resources

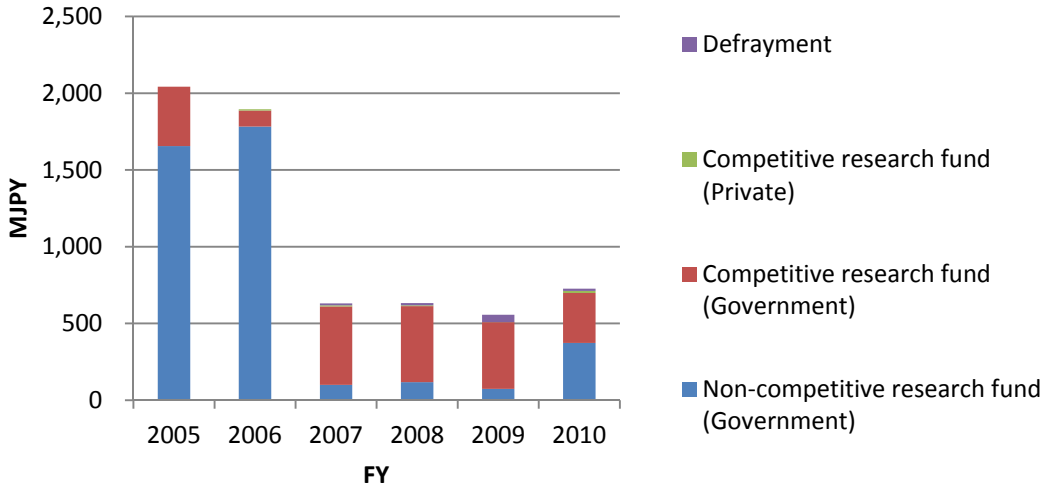
2-2-1. Government Funds



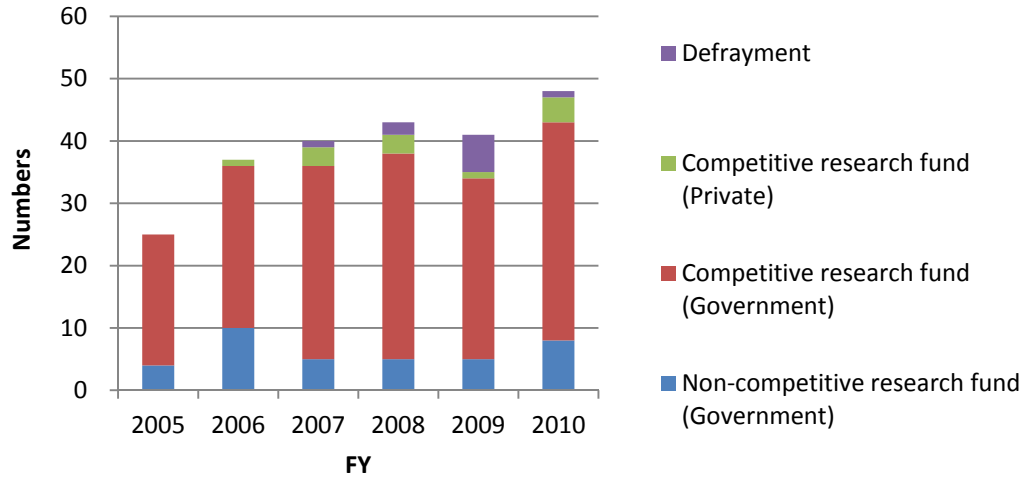
2-2-2. External Funds

The RSC has also actively competed over the years in bidding for research grants, subsidies and commissions from MEXT, various other government ministries and agencies, and other public corporations commissioning and outsourcing research.

The Acquisition of External Funds (JPY)

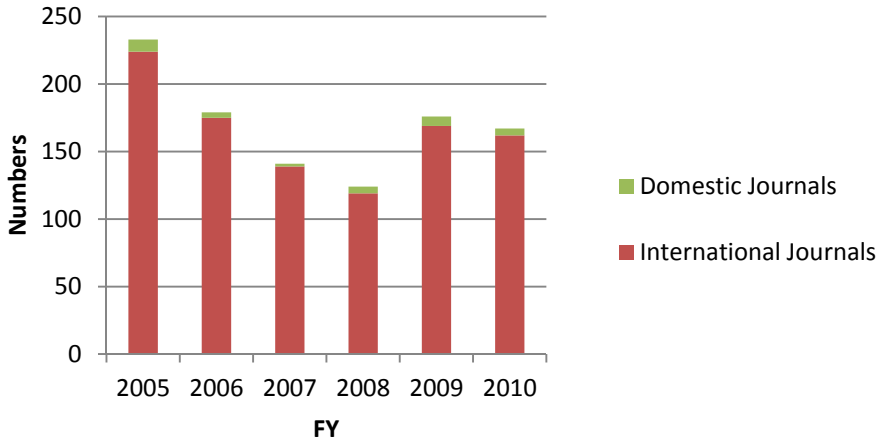


The Acquisition of External Funds (numbers)

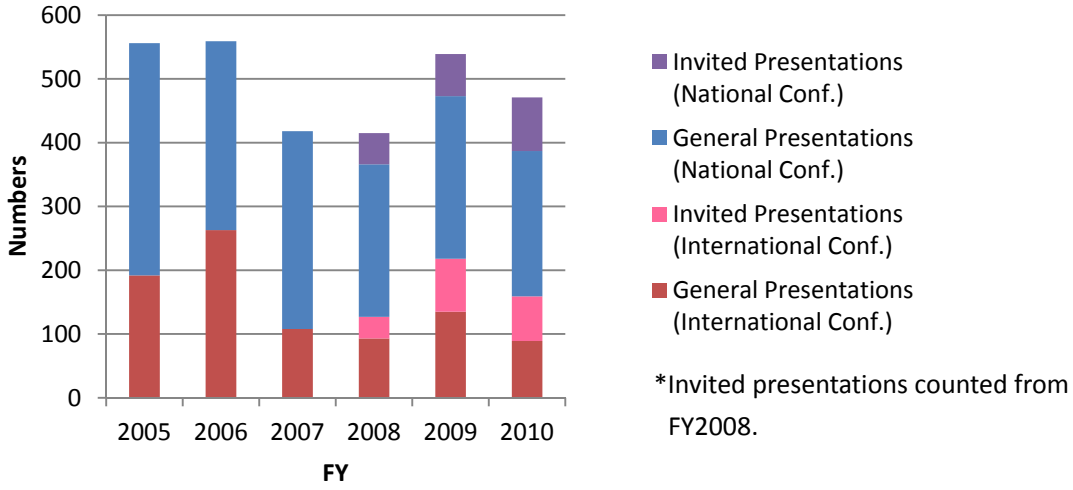


2-3. Research Output

2-3-1. Number of Original Research Papers

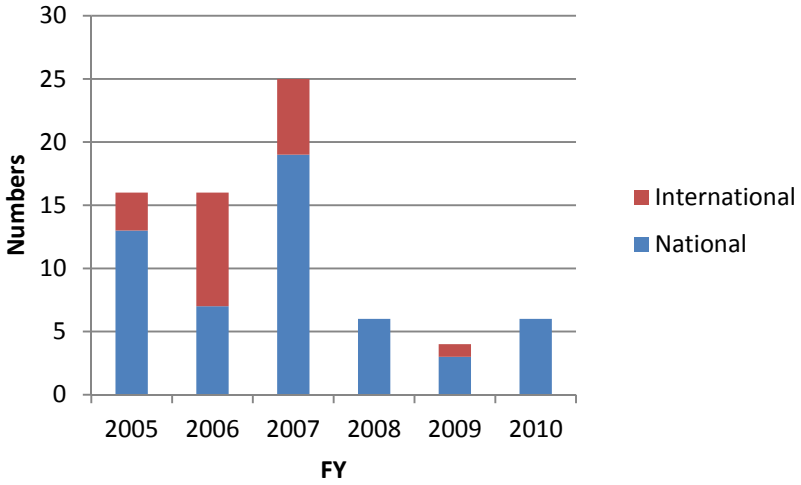


2-3-2. Number of Presentations



2-3-3. Intellectual Property

Numbers of Patent Applications



Registered Patent List

Registered Date	Registration No.	Title	Country
Jan 5, 2007	3898667	METHOD AND INSTRUMENT FOR DETECTING PROTEIN CRYSTAL, AND PROTEIN CRYSTAL DETECTING PROGRAM	Japan
May 23, 2008	4127329	POLARIZATION GENERATING DEVICE AND ASSEMBLY JIG THEREOF	Japan
Jan 30, 2009	4251648	UNDULATOR	Japan
Jul 10, 2009	4338575	PREPARATION METHOD OF HEAVY ATOM DERIVATIVE USING VAPORIZED IODINE, METHOD FOR COLLECTING PHASE INFORMATION, AND METHOD FOR DETERMINING THREE-DIMENSIONAL STRUCTURE OF PROTEIN CRYSTAL	Japan
Jul 24, 2009	4347966	REVOLVER TYPE INSERTION LIGHT SOURCE	Japan
Sep 30, 2009	1754716	Extreme thermophile single-stranded DNA binding mutant protein, and nucleic acid isothermal amplification method of use thereof	Germany, France, UK
Apr 2, 2010	4482688	MAGNETIC FIELD GENERATING METHOD AND MAGNETIC FIELD GENERATOR	Japan
Aug 3, 2010	7770232	Scanning probe microscope system	USA
Oct 29, 2010	4613289	MAGNETIC FIELD GENERATING METHOD AND MAGNETIC FIELD GENERATOR	Japan
Jan 18, 2011	7872555	Undulator	USA
Feb 25, 2011	4691144	ELECTRONIC APPARATUS STORING RACK	Japan

2-3-4. International Symposiums

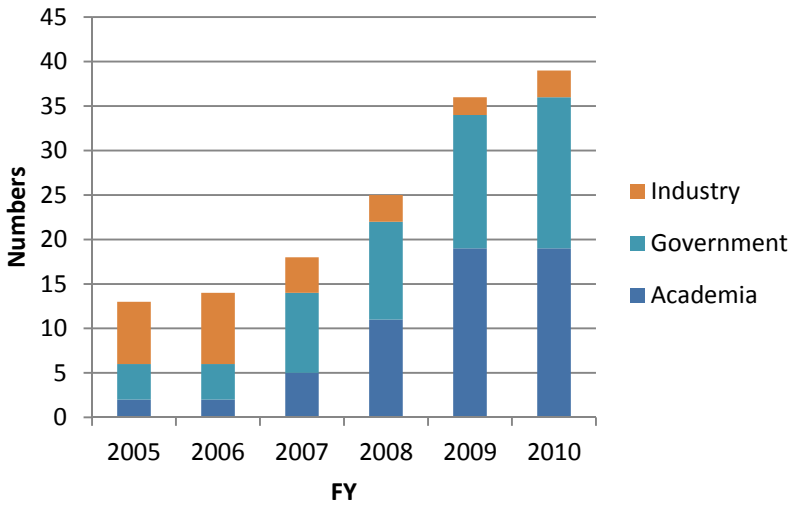
Date	Title	Venue
Nov 15-17, 1999	International Workshop for the Use of 30m Long Super Brilliant Undulator X-rays	Center for Advanced Science & Technology (CAST), Harima
Apr 9-12, 2000	The 6th SPring-8, ESRF, APS Workshop	SPring-8, Harima
Jul 9-10, 2000	2nd UK-Japan Int. Seminar on Applications of Synchrotron Radiation to Studies of Nano-Structured Materials	SPring-8 Public Center, Harima
Jul 26-31, 2000	11th Int. Conf. on X-Ray Adsorption Fine Structures (XAFS IX)	Ako Harmony Hall, Hyogo
Nov 7-8, 2000	Harima Workshop on Implementation for High-throughput Structure Determination by Protein Crystallography	SPring-8 Public Center, Harima
Nov 9-10, 2000	UK-Japan (DL/RIKEN/JASRI) Joint Symposium	SPring-8 Main Building Lecture Room, Harima
May 1-4, 2002	24th Advanced ICFA Beam Dynamics Workshop on Future Light Sources	SPring-8, Harima
May 10-12, 2002	5th SPring-8 Int. Workshop on 30-m Long Straight Sections	SPring-8, Harima
Aug 22-26, 2002	Int. Workshop on Photoionization (IWP2002)	SPring-8, Harima
Oct 15-16, 2002	5th SRRTNet Workshop on the Interface between Theory, Computation and Experiments	SPring-8, Harima
Jan 14-15, 2004	The Third CCLRC-JASRI Symposium	SPring-8, Harima
Sep 7-11, 2004	8th International Conference on Biology and Synchrotron Radiation (BSR2004)	Egret Himeji, Himeji
Nov 8-10, 2004	The 9th SPring-8, ESRF, APS Workshop	Spring-8
May 28-30, 2005	2nd Bilateral Japan-UK Symposium	RIKEN Yokohama Institute
Nov 8-1, 2005	Tri-Party (SPring-8, ESRF, APS) Optics Workshop	
Nov 17-19, 2005	3rd International Workshop on Radiation Safety Synchrotron Radiation Sources	
Mar 7-8, 2006	4th International Workshop on X-ray Damage to Biological Crystalline Samples	SPring-8 Public Center, Harima
Apr 14-15, 2006	CHEMICAL BIOLOGY OF REDOX METALLOENZYMES Post Symposium of “The 50th Anniversary of Oxygenases – Advances and Reflections –“	
Oct 27-28, 2006	The 7th Japan-Korea-Taiwan Symposium on Strongly Correlated Electron Systems	SPring-8 Public Center, Harima
May 7-11, 2007	6th International Conference on Inelastic X-ray Scattering	Awaji Yumebutai International Conference Center, Awaji Island
Oct 21, 2007	The 2nd X-ray Free Electron Laser Symposium	Center for Advanced Science & Technology (CAST), Harima

Date	Title	Venue
Jan 22, 2008	The 3rd X-ray Free Electron Laser Symposium	Marunouchi MY PLAZA Hall, Tokyo
Feb 26, 2008	SPring-8 GPCR Symposium	SPring-8 Public Center, Harima
May 21-22, 2008	3rd International Conference on Diamonds for Modern Light Sources	Awaji Yumebutai International Conference Center, Awaji Island
Dec 12, 2008	The 4th X-ray Free Electron Laser Symposium	International Exchange Center , Tokyo
Feb 16-18, 2009	The 1st Workshop on FEL Science "Coherent Intense X-rays in Physics and Biology"	Jeju, Korea
Jun 19, 2009	SPring-8II 2019 Symposium	Tokyo Station Conference
Oct 5-6, 2009	Workshop on POSTECH-RIKEN Joint Research Program	
Nov 27, 2009	The 5th X-ray Free Electron Laser Symposium	Shinagawa Intercity Hall, Tokyo
Dec 6-9, 2009	The 2nd Workshop on FEL Science: "Emerging X-ray Applications in Biological Systems"	Pingtung Hsieng, Taiwan
Jan 9, 2010	Science lecture for citizens	Himeji
Apr 12-14, 2010	The 12th SPring-8, ESRF, APS Workshop	SPring-8, Harima
Sep 4, 2010	The 6th X-ray Free Electron Laser Symposium	Umeda Center Building, Osaka
Oct 4-7, 2010	The 3rd Workshop on FEL Science “Emerging X-ray Applications in Biological Systems-II”	Kitayuzawa, Hokkaido, Japan
Nov 20, 2010	SPring-8 Special Symposium -Synchrotron radiation light on cultural properties and Histories-	New Public Hall, Nara
Dec 4, 2010	The 2nd SPring-8II 2019 Symposium	Gakujyutu-sogo Center, Tokyo
Dec 7-10, 2010	GPCR Workshop 2010	Honolulu, Hawaii
Feb 12-13, 2011	Workshop on Structural Biology in Southern Taiwan through RIKEN PTP	Taiwan
Mar 26, 2011	2nd Science Lecture for Citizens	Himeji Citizen Hall, Hyogo

2-4. Collaboration

2-4-1. Domestic Organizations

Number of Collaborations with Domestic Organizations

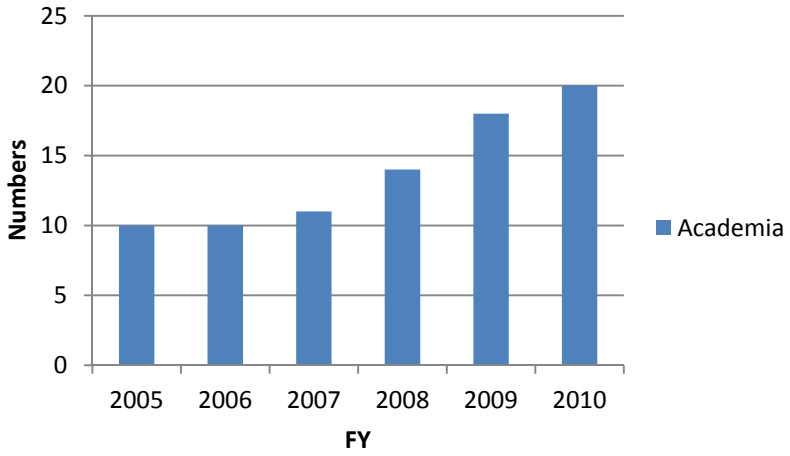


List of Collaborations with Domestic Organizations (FY2010)

Type	Organization
Academia	Hokkaido University, Tohoku University, Iwate university, Keio University, Utsunomiya University, The University of Tokyo, The University of Electro-Communications, Kyoto University, Osaka University, Kobe University, University of Hyogo, Tottori University,
Government	Technology Research Association Fuel Cell Cutting-Edge Research Center FC-Cubic, Japan Biological Information Consortium, High Energy Accelerator Research Organization (KEK), National Institute of Natural Science, Japan Aerospace Exploration Agency, National Institute of Advanced Industrial Science and Technology, Japan Synchrotron Radiation Research Institute, National Research Institute of Fisheries and Environment of Inland Sea, Fisheries Research Agency, Japan Atomic Energy Agency, National Agriculture and Food Research Organization
Industry	OKI Semiconductor, Rigaku, J-Tech

2-4-2. Foreign Organizations (based on written agreements)

Numbers of Collaborations with Foreign Organizations



List of Collaborations with Foreign Organizations (FY2010)

For Third-Generation Synchrotron Radiation Facilities

Country	Organization	Details	Started-
USA	Advanced Photon Source, Argonne National Laboratory (DOE, APS)	Synchrotron radiation research	1993
France	The European Synchrotron Radiation Facility (ESRF)		

For XFEL

Country	Organization	Details	Started-
USA	Stanford Linear Accelerator Center (SLAC)	Free Electron Laser (FEL)	2006
Germany	The Deutsches Elektronen-Synchrotron (DESY)		

Others

Country	Organization	Details	Started-
Korea	Pohang Accelerator Laboratory (PAL)	synchrotron radiation research**	2005
	Gwangju Institute of Science and Technology (GIST) / Center for Extreme Light Applications (CELA)	Coherent X-ray technology	2010
Taiwan	National Synchrotron Radiation Research Center (NSRRC)	Synchrotron radiation research**	2008
Thailand	National Synchrotron Research Canter	Synchrotron radiation research	2006
India	Indian Institute of Science(IISc)	Coherent X-ray technology	2011

Country	Organization	Details	Started-
Australia	Australian Synchrotron	Synchrotron radiation research**	2008
	ARC Centre of Excellence for Coherent X-ray Science of The University of Melbourne	Coherent x-ray technology	2010
USA	Lawrence Berkley National Laboratory (LBNL)	Production and installation of an in-vacuum insertion device	2004
	Advanced Photon Source, Argonne National Laboratory (DOE, APS)	Synchrotron radiation research**	2006
	ARGONNE NATIONAL LABORATORY (ANL)	X-ray Free Electron Laser-Oscillator	2009
	Brookhaven National Laboratory (BNL) NSLSII	Synchrotron radiation facility and instrumentation development**	2009
UK	Daresbury Laboratory/ Council for the Central Laboratory of Research Councils (CCLRC)	Bimolecular and physical sciences	2000
	DIAMOND Light Source Ltd.	Synchrotron radiation research**	2006
Germany	The Deutsches Elektronen-Synchrotron (DESY)	Synchrotron radiation research**	2007
Denmark	The Center for Materials Crystallography, Aarhus University	Synchrotron radiation research	2010
Switzerland	Paul Scherrer Institute (PSI)	Development of in-vacuum undulators**	2006

**Three-way agreement with JASRI

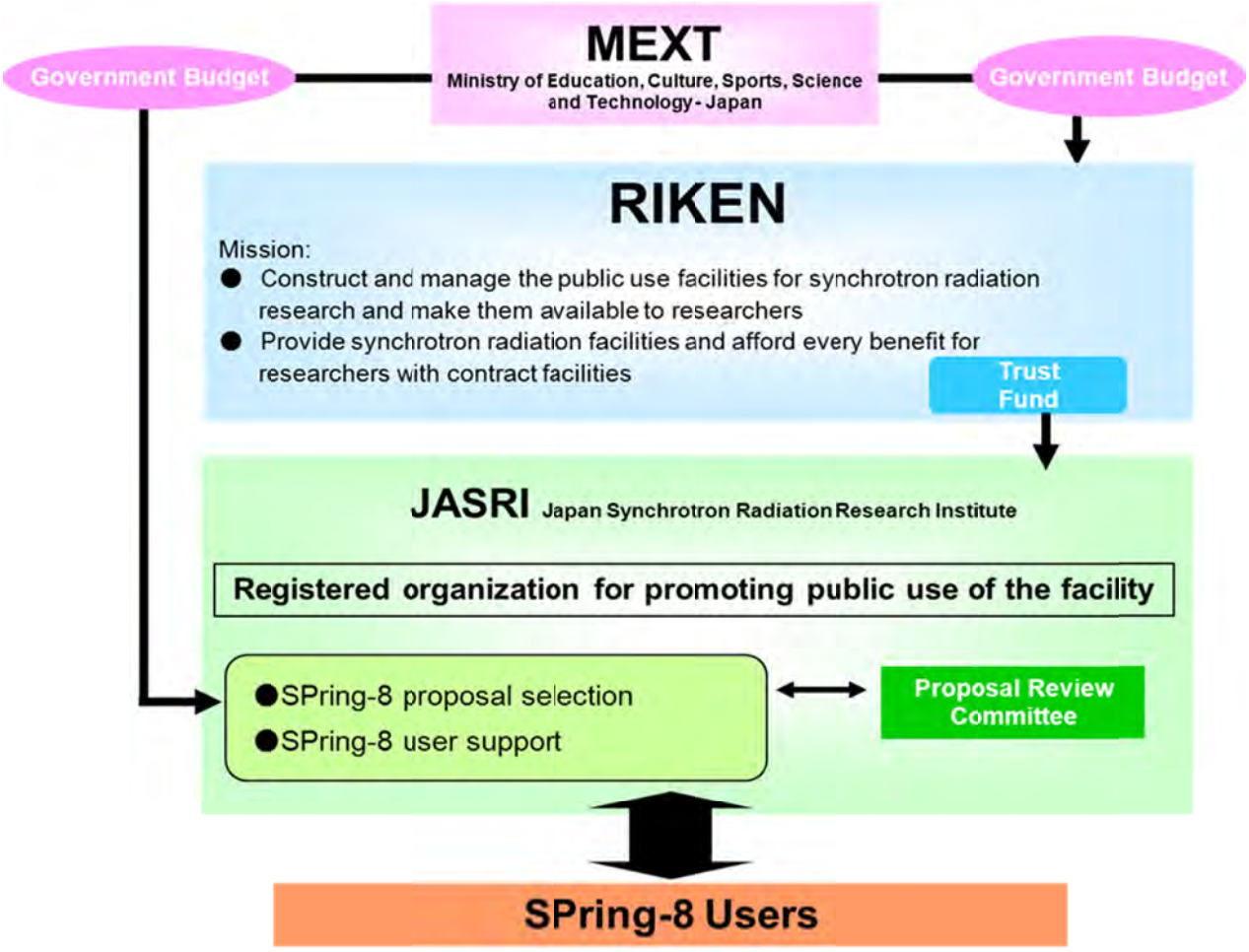
3. SPring-8

3-1. Management of SPring-8

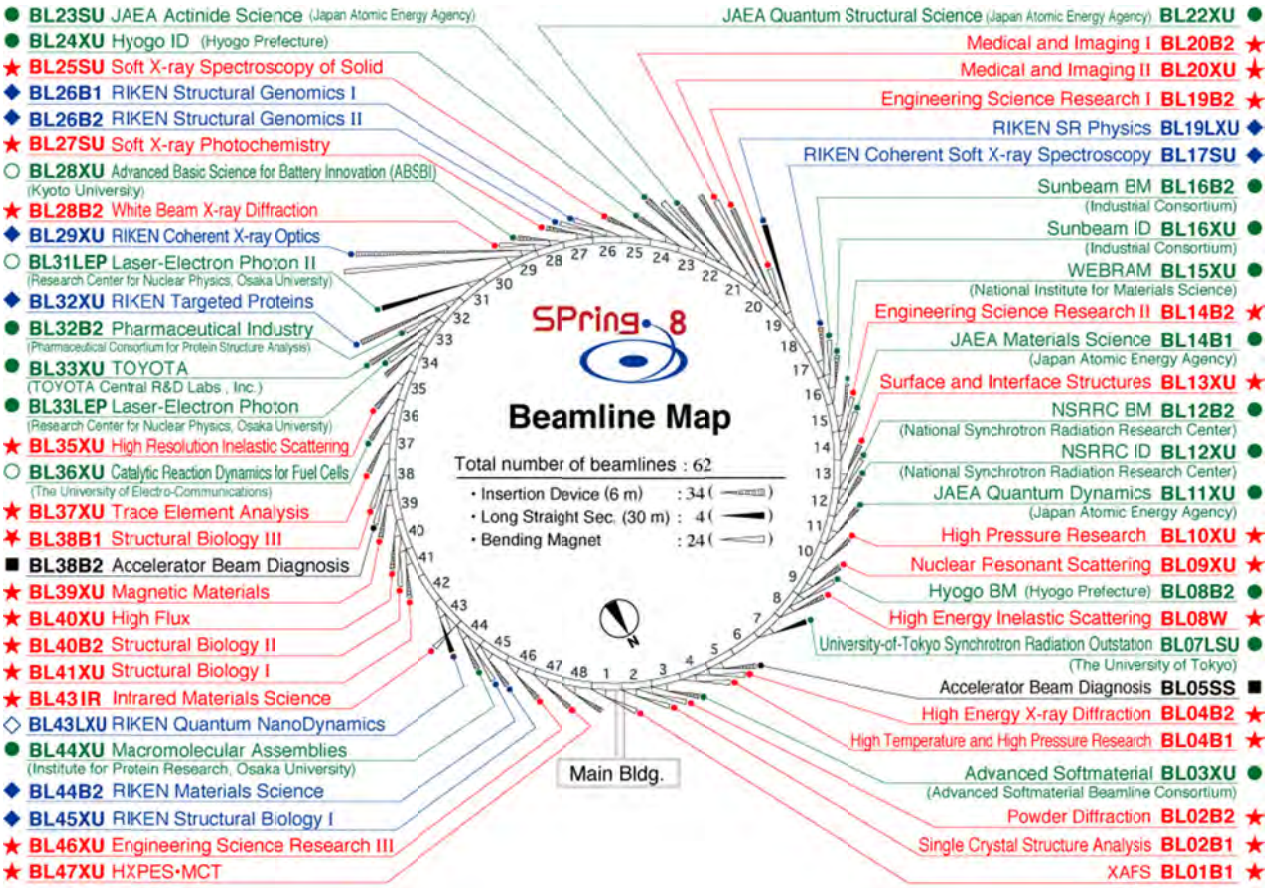
When the construction of the SPring-8 facility started in 1991, both RIKEN and JAERI (now the Japan Atomic Energy Agency, or "JAEA") were the owners of SPring-8. In 1994, JASRI was designated as a national organization with a mission of promoting public use of the Synchrotron Radiation Facility (SPring-8). JASRI was commissioned both by RIKEN and JAERI to operate, maintain and upgrade the facility.

The first beam was produced radiation in 1996 and SPring-8 was opened to the public in 1997.

JAERI withdrew from the project at the end of September 2005, leaving only JASRI commissioned by RIKEN. In 2006, the Japanese law enacted for "the promotion of public use of the Synchrotron Radiation Facility (SPring-8)" was amended to promote "public use of advanced large research facilities." Under the new law, the designated organization system was changed to a registered organization system, which altered the relationship between RIKEN and JASRI. Consequently, as the sole owner of SPring-8, RIKEN was obligated to bear more management responsibility.



3-2. Beamlines of SPring-8



BL: Beamline
B1, B2: Bending Magnets
XU: X-ray Undulator
SU: Soft X-ray Undulator
W: Wiggler

IR: Infrared Radiation
LEP: Laser-Electron Photon
LXU: Long-length X-ray Undulator
LSU: Long-length Soft X-ray Undulator
SS: Straight Section

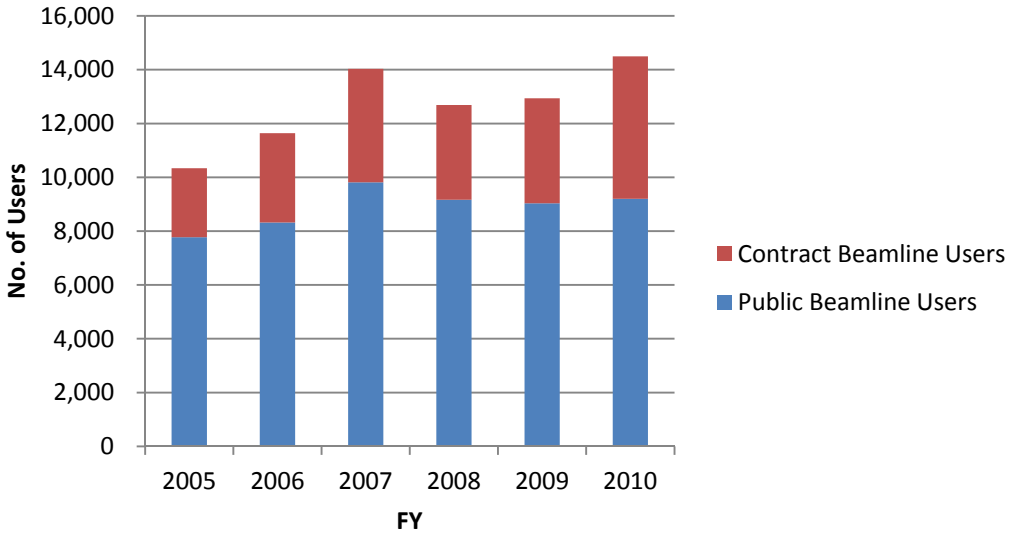
WEBRAM: Wide Energy Range Beamline for Research in Advanced Materials
NSRRC: National Synchrotron Radiation Research Center, Taiwan

★ : Public Beamlines
● : Contract Beamlines
◆ : RIKEN Beamlines
■ : Accelerator Diagnostics Beamlines
☆ ○ ◇ □ : Planned or Under Construction

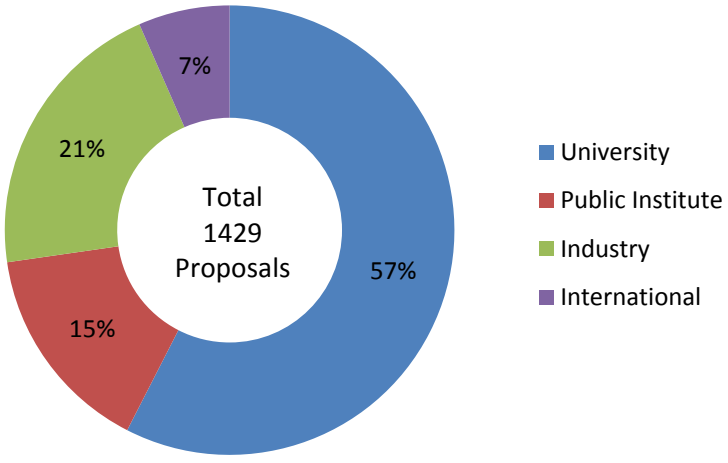
August 9, 2010

3-3. Status of SPring-8 Users

3-3-1. Numbers of SPring-8 Users



3-3-2. Representative Affiliations for Approved Proposals



4. The XFEL Project

The XFEL (X-ray Free Electron Laser) of the national project began in March 2006 with a five-year-plan and the RIKEN XFEL Head Office was launched. The following month, RIKEN and JASRI established a joint promotion office for the XFEL project to aim for the construction of the XFEL facilities adjacent to SPring-8. The project completed in March 2010 and the first lasing was achieved in June 2011. One of the main missions of the RSC is to operate, manage, maintain and promote full use of the XFEL facility.

Apr 2000	The XFEL development concept; compact and low-cost was drafted
Jan 2002	In-vacuum undulator with a shorter period and higher magnetic field was completed
Dec 2003	Electron gun was completed, a world record for its emittance value was achieved
Nov 2004	R&D group for the XFEL in RIKEN was launched
Jan 2005	The XFEL project was designated as an important research objective for future R&D in the Ministry of Education, Culture, Sports, Science and Technology (MEXT) policy report on promoting science and technology of light and photons
Feb 2005	The International Review Committee Meeting for XFEL was organized and was recommended to promote the XFEL project
May 2005	The conceptual design report on SPring-8 Compact SASE Source (SCSS, the XFEL prototype), was released
May 2005	XFEL user promotion group was launched
Sep 2005	MEXT working group for the next-generation synchrotron light source project reviewed and reported on the XFEL to carry actively forward
Nov 2005	First synchrotron radiation was observed at the SCSS
Dec 2005	12.4 billion JPY for the first National Budget to start constructing XFEL and its R&D was allocated by Japanese Government
Feb 2006	The first recommendation of the RIKEN SPring-8 Center Advisory Council (RSAC) for the RIKEN Harima Institute to increase its responsibility for both XFEL and SPring-8 facilities and the RSC to focus on the design and use of the world-leading photon sources was presented
Mar 2006	The XFEL Project Head Office was launched
Apr 2006	The SPring-8 Joint Project for XFEL was established by RIKEN and Japan Synchrotron Radiation Research Institute (JASRI)
Jun 2006	First Lasing at the SCSS was achieved
Nov 2006	The 1st XFEL Symposium
Jul 2007	Construction of the XFEL facility began
Sep 2007	Full-lasing of the SCSS in 50-61nm wavelength was achieved
Oct 2007	The 2nd XFEL Symposium
Jan 2008	First call for the User Projects of the SCSS
Jan 2008	The 3rd XFEL Symposium
Dec 2008	The 4th XFEL Symposium
Mar 2009	Construction of the accelerator building and the undulator building was completed
Apr 2009	Installation of electron gun, acceleration tubes, undulators began

Nov 2009	The 5th XFEL Symposium
May 2010	Construction of experiment/research building was completed
Mar 2011	The XFEL facility was named 'SACLA'. First synchrotron radiation was observed
Jun 2011	First Lasing at SACLA was achieved
in 2012	SACLA's operation for public use will start

APPENDIX Ⅱ
RIKEN

1. History of RIKEN

1-1. RIKEN Foundation (1917-48)

RIKEN was established initially as a private foundation independent of the government, and by developing large-scale laboratories, RIKEN contributed to raising the competitiveness of Japan's scientific research to the level of overseas research institutions.

In 1916, the organizing committee for the founding of the RIKEN Foundation distributed a document titled "RIKEN and Industry." This document had emphasized not only applied research directly linked to economic development, but also the necessity of laboratories conducting basic research in physics and chemistry. The outbreak of World War I disrupted the import of resources from various countries. This led to the proposal to establish RIKEN for the purpose of raising Japan's national strength, and in particular its science and technology to an international level, attracted capital from the imperial household, government and the industrialists. On March 20, 1917, RIKEN was officially established.

In 1922, Prof. Masatoshi Okochi, the third President of RIKEN, introduced a new system for organizing research. Chief Scientists were appointed to direct the laboratories and given substantial autonomy in conducting the affairs of their own research topics. RIKEN permitted its Chief Scientists to have joint appointments with universities as professors, and this gave rise to RIKEN's tradition of maintaining close ties with academia.

Shortly after its establishment, economic hardships confronted RIKEN. As a countermeasure, RIKEN reinforced its position by licensing achievements transferable to industry as commercial products to industry. RIKEN began developing close ties with affiliated industries in 1927, and by 1941 had licensing affiliations with 63 companies and 121 factories. The dividends and patent utilization fees from these companies became an indispensable source of RIKEN's income.

World War II cast a dark shadow over RIKEN's future. RIKEN lost two-thirds of its buildings to war, and almost all of its facilities suffered bomb damage. After the war, the general headquarters (GHQ) of the occupying forces issued a verdict that RIKEN was a zaibatsu (a financial conglomeration) that should not be allowed to continue. RIKEN had no choice but to sever its ties with the affiliated companies.

1-2. Scientific Research Institute Ltd. (Kaken: 1948-58)

In 1947, the government enacted a law to reorganize the RIKEN Foundation as a stock corporation named Scientific Research Institute Ltd., or Kaken for short in Japanese. In accordance to the law, private-sector industries became shareholders of the intellectual assets and physical resources provisioned from the former RIKEN Foundation, and the foundation's operation as Kaken began in 1948. Kaken's efforts to conduct research contributing to the revival of Japanese industry collapsed, however, due to fiscal hardships. In 1952, the applied manufacturing technology segment was separated from the research segment to begin Kaken's second phase of existence. But this restructuring did not resolve Kaken's financial crisis, and in 1955 the government had to step in with assistance.

1-3. RIKEN's Structural Transition (1958)

Kaken's third phase of existence as a government-assisted corporation also failed in resolving the financial problems. The government concluded from discussions in 1957 that Kaken was not viable on a commercial basis. As an alternative measure, the government enacted the Institute of Physical and Chemical Research (RIKEN) Law, and Kaken was converted to a public corporation under the umbrella of the Science and Technology Agency to be once again named RIKEN in 1958.

Article 1 of the RIKEN Law：
The purpose of RIKEN shall be to comprehensively conduct research and experimentation of science and technology (excluding research pertaining solely to humanities) and disseminate the achievements.

In March 1959, RIKEN's Board of Executive Directors decided the institute's basic management policies as

follows:
a) Give laboratories autonomy under the leadership of the Chief Scientists in accordance with the RIKEN Foundation system.
b) Organize a Chief Scientist's Assembly as an advisory body to the President, to allow researchers to have an active role in the research and management policies of the institution.

1-4. Growth of RIKEN as a Public Corporation (1958-2003)

Most of RIKEN's laboratories and research facilities were relocated between 1966 and 1968, from the founding grounds of Komagome in central Tokyo, to a spacious 25-hectre campus 40 minutes by train from Tokyo in Wako City, Saitama Prefecture. The move enabled major expansion of the research facilities.

In 1984, RIKEN opened the Tsukuba Life Science Research Center in response to the government's policy based on the Council for Science and Technology recommendations for promoting life science research.

RIKEN's cutting edge and groundbreaking Frontier Research Program (FRP) began in 1986 in accordance with the government's initiative to secure Japan's superiority in leading-edge science and technology. The mandatory retirement age system by a single employer was the norm in Japan at that time, but the FRP proved that noteworthy achievements could result from giving limited term contracts to first-rate researchers from within Japan and across the world for participating in frontier research projects. RIKEN's principal motive in jointly establishing new research centers with local municipal authorities in Sendai (1990) and Nagoya (1993) was also to further the expansion of the FRP system.

Meanwhile, RIKEN, in an effort to collaborate with another public corporation, joined hands with the Japan Atomic Energy Research Institute in 1988 to begin design and construction of SPring-8, a synchrotron radiation research facility. When the laboratory became operational in 1997, it became the world's most powerful third-generation synchrotron radiation accelerator. SPring-8 received industrial, governmental and academic support right from inception, and a great deal of assistance in making the project a success from Hyogo Prefecture in particular.

RIKEN's first overseas research laboratory was established in April 1995. The Muon Science Research Laboratory located at Great Britain's Rutherford Appleton Laboratory has long been the cornerstone of joint research between the two nation' institutes.
Success of this facility led to the opening of the RIKEN-BNL Research Center in New York, RIKEN's second overseas laboratory, under the guidance of Nobel Prize laureate Prof. T.D. Lee in 1997.

SPring-8's capacity to perform world-class research, such as structural biology, quickly attained international renown. The RIKEN Harima Institute was established for the purpose of fully exploiting this technology to begin operations alongside the synchrotron ring in October 1997.

The RIKEN Brain Science Institute (BSI) was established in October 1997 to amalgamate and advance some of the research activities that had already been underway in the FRP. The BSI's goal is to become not only the center of research in Japan for brain science, but also an international "center of excellence."

In October 1998, RIKEN established the Genomic Sciences Center (GSC) with the aim of making it Japan's hub for genomic research. Three laboratories (genomic science, cell signaling and plant molecular biology) directed by chief scientists in the life science field were consolidated at the center in cooperation with the University of Tokyo and the National Institute of Genetics. Shortly after, the GSC was relocated to the RIKEN Yokohama Institute that opened in April 2000.

RIKEN in April 2000 established the Plant Science Center (PSC) and the Single Nucleotide Polymorphism (SNP) Research Center as part of the Yokohama Institute. Along with the increase in the number of RIKEN's research centers, the Tsukuba Life Science Research Center was renamed the Tsukuba Institute and remade a Center for Developmental Biology.

In January 2001, a BioResource Center was established within the Tsukuba Institute, to begin undertaking the inventory and distribution of biological resources that until then had been maintained phyletically by separate

institutions within Japan and abroad. In July, the Research Center for Allergy and Immunology was established as the fourth research center to be located at the Yokohama Institute.

In April 2002, laboratories directed by Chief Scientists at the Wako Campus were consolidated into the RIKEN Discovery Research Institute. The Kobe Institute was also opened in Kobe City, and the Center for Developmental Biology was relocated there. In December, the Nanoscience Research Program (NRP) was inaugurated to add flexibility in responding to the highly scholastic demands in the field of nanoscience research.

After having grown and produced results as a public corporation, RIKEN's status as such was dissolved at the end of September 2003, following the Japanese government's decision to dissolve and consolidate its public corporations.

1-5. RIKEN as the Independent Administrative Institution (2003-)

On October 2003, RIKEN's status changed from that of a public corporation to that of an Independent Administrative Institution. Independent Administrative Institutions are enterprises that draft their own mid-term plans based in principle on a five-year target the government proposes. They need to receive approval from the relevant government ministers for carrying out their plans.

Soon after becoming an Independent Administrative Institution, RIKEN's research functions at the Wako Main Campus were reorganized as the Wako Research Institute, and the administrative headquarters functions were separated as the Wako Headquarters.

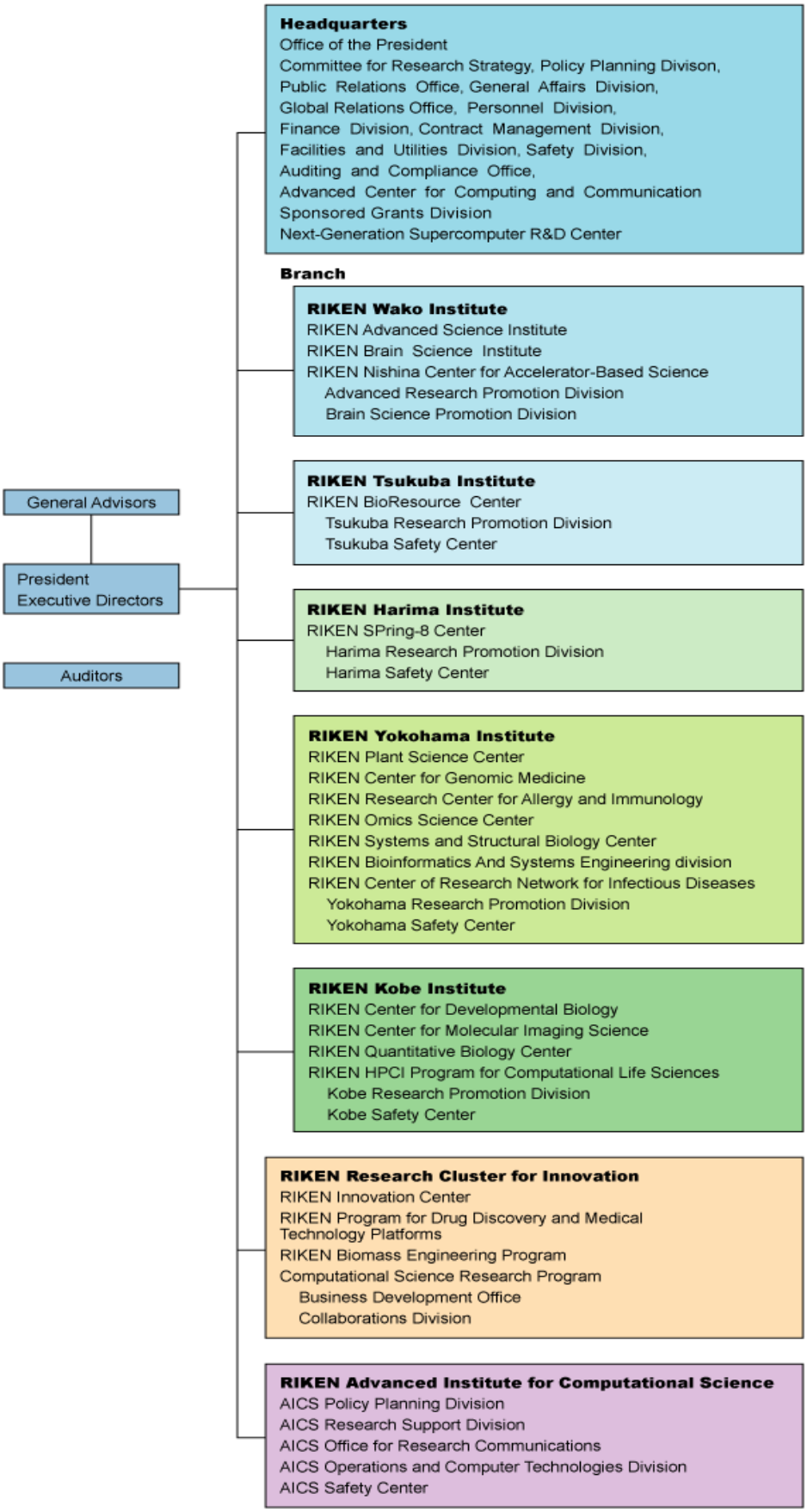
Nobel Prize scientist Prof. Ryoji Noyori assumed the post of the Independent Administrative Institution's first President and since then has been managing RIKEN in accordance with the five policy initiatives he proposed known as the Noyori Initiative (see section 2-2. Noyori Initiative).

2. Management of RIKEN

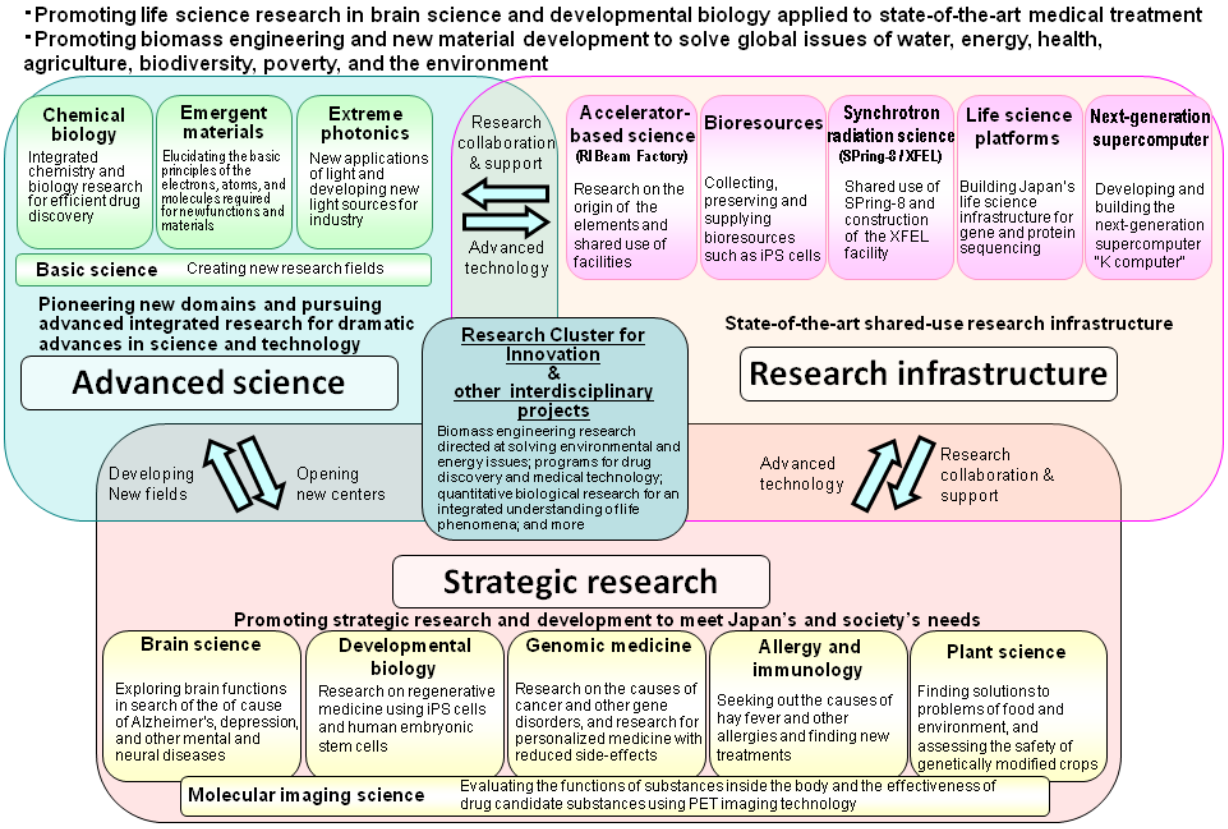
2-1. RIEKN's role in Advancing Japan's Science and Technology Policies

2-1-1. Organizational Structure of RIKEN

as of April 2011



2-1-1. RIKEN Research System



2-2. Noyori Initiative

Dr. Ryoji Noyori became the president of RIKEN in October 2003 when RIKEN was reorganized as an Independent Administrative Institution. Dr. Noyori immediately announced the Noyori Initiative, guidelines describing his vision on strategy and management, for all staff in RIKEN.

1. Visibility of RIKEN
- Improve the image and public awareness of RIKEN
- Researchers and administrative staff should make the public aware of the importance of science and technology

2. Maintaining RIKEN's Outstanding History of Achievement in Science and Technology
- Sustain and develop the RIKEN research spirit
- Emphasis on quality of research. Sustain exceptional prestige of the RIKEN brand
- Further strengthen the realization of intellectual property to make contributions to society and industry

3. RIKEN that Motivates Researchers
- Curiosity-driven concepts
- Posing the problem of uniqueness and high risk
- Fostering promising human resources

4. RIKEN that is Useful to the World
- Close ties with industry and society
- Science and technology that support civilized society (beyond the means of universities or industry)

5. RIKEN that Contributes to Culture
- RIKEN must raise the level of its own culture
- Dissemination of knowledge to humanities and social science

2-3. Midterm Goals and Evaluations

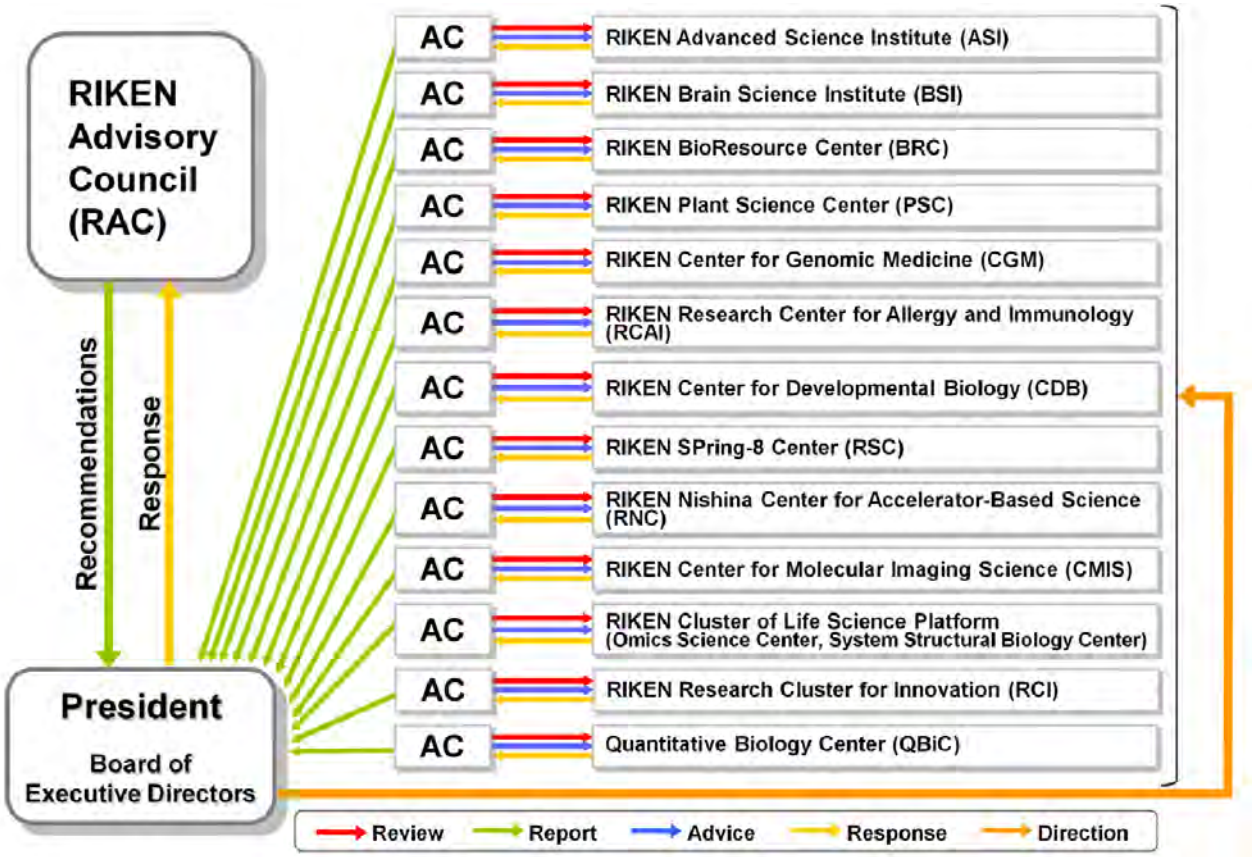
2-3-1. Midterm Goals

The Japanese government draws up Midterm Goals for a specified five–year periods. Each independent administrative institution must then draw up and get approval of a corresponding Midterm Plan to accomplish the goals. The first Midterm ran from October 2003 to March 2008. The second Midterm runs from April 2008 to March 2013.
For the second Midterm, the missions of the RSC are “to maintain SPring-8 and the X-ray Free Electron Laser as the world’s best research facility and to provide tools and know-how for internal and external RIKEN researchers at the Japanese Center of Excellence in photon science.”

2-3-2. RAC (RIKEN Advisory Council)

RIKEN has been internally reviewing its projects since 1965 and reviewing the research achievements of the Institute Laboratories since 1982. The RAC (the RIKEN Advisory Council) has convened since 1993 to provide advice and recommendations to the President of RIKEN about basic issues regarding its research activities and management. RIKEN’s pioneering efforts on the review system led to the framework of the evaluation guidelines from the government. RIKEN has used the review results to improve management as well as to enact other specific measures.

RIKEN currently has thirteen research centers, each with its own Advisory Council. All of the Advisory Council chairpersons from these research centers are required to participate in the RAC.



2-3-3. RSAC (RIKEN SPring-8 Center Advisory Council)

The RSAC is an advisory council for the RIKEN Spring-8 Center (RSC). The Director of the RSC and the President of RIKEN ask the RSAC to consider and provide feedback on fundamental management issues and research activities. RSAC meetings are held twice during each Midterm (five year period). The last RSAC was held in February 2009 (see APPENDIX III).

2-3-4. Independent administrative institution (IAI) assessment

Every Independent Administrative Institution (IAI) should be assessed both annually and at the end of the Midterm. In the last IAI assessment (June 2010), the committee made the following recommendations regarding the RIKEN Harima Institute:

It is necessary to revise SPring-8 operation systems and consignment contracts consistently in order to be in an effective and efficient manner.

APPENDIX Ⅲ

RIKEN SPring-8 Center Advisory Council (RSAC) 2009

1. Report on RSAC 2009

Date: February 8 - 10, 2009

AC members:

Jerome B. Hastings (Chair)	Professor, SLAC National Accelerator Laboratory
Osamu Shimomura (Vice Chair)	Executive Director, KEK (High Energy Accelerator Research Organization)
Sunggi Baik	President, POSTECH (Pohang University of Science and Technology)
Sine Larsen	Director of Research, ESRF (European Synchrotron Radiation Facility)
Keiichi Namba	Professor, Osaka University

General Statement

The RIKEN SPring-8 Center (RSC) plays many important roles in the frontiers of science and technology, from the materials science to the life science fields, by providing state-of-the-art experimental facilities utilizing brilliant light sources as well as by promoting its own research activities. A rather drastic turnover of many PIs and reorganization of the RSC to a more mission-oriented structure with three divisions in response to the 1st RSAC-2006 recommendations proved to be quite a challenge. But, together with RIKEN's new mission of constructing a compact XFEL facility by the end of FY 2011, the three divisions of the RSC have been actively fulfilling their assigned responsibilities. The Innovative Light Sources Division is responsible for the technical development of advanced SR sources including XFEL; the Photon Science Research Division carries out cutting edge research in life, materials and physical sciences at SPring-8; and the Advanced Photon Technology Division is developing technologies to make the best use of SPring-8 and XFEL for users, including scientists from the industrial sectors. Construction for the XFEL facility is now well advanced - it is to be completed in about two years as originally planned. The recent achievements, present activities and future plans by groups in each of the three divisions have proved the RSC to be one of the leading institutes in the world, with impressive progress and exciting potential as described by individual PIs at the RSAC 2009. It is crucial to maintain and to further improve the quality and level of R&D for the RSC to continue to be a leading figure in the world scientific community and to contribute to the future developments of industrial and medical science and technology. The RSC's mission to contribute to the benefit of human society is indeed a formidable challenge.

Comments on Specified Issues

1. **The management system of the RIKEN SPring-8 Center, especially its organizational structure and administrative systems, and its aim of making the RSC a world-leading research institute.**

The RSC reorganized in response to the RSAC-2006 recommendations. Reorganizations are always difficult and the RSC stepped up to the challenge. The new mission-oriented structure is working well as evidenced from the comments below about scientific progress and impacts. That being said, there remains a challenge ahead: to provide scientific leadership for use of the XFEL. The XFEL will begin operation in just over two years and the recruitment of staff and the establishment of new laboratories and/or the re-direction of existing staff and laboratories needs to be completed in a very short time. The approach to this challenge should engage the ultra-fast science community in Japan and take advantage of the scientific leadership that is already part of RIKEN (e.g., the independent laboratory of Dr. Midorikawa).

The RSC also needs to expand the role of the advanced photon technology division to include the XFEL. Only then can the value of the developments for both storage ring and FEL experiments be completely realized. These unique opportunities present corresponding challenges. The structure of a mission-oriented organization provides a good platform to meet these challenges, but it needs to be nimble and able to adapt quickly. It will require strong leadership and cooperation, but the RSC has shown that it is prepared to meet this challenge.

To keep and retain a vibrant research community on the SPring-8 campus it is critical to have a significant

number of young scientists, students and postdoctoral researchers. The RSC should make a serious effort to understand how to attract additional young research staff and graduate students to the SPring-8 campus to get them involved in its world-top level research activities. The number of postdoctoral fellows and graduate students appears to be rather limited, but the potential opportunities for such young people are tremendous. Working with these young people will also stimulate discussion within the SPring-8 community, among groups of different expertise and disciplines and spanning generations. The isolated location of the campus may make the SPring-8 campus less attractive to young people, as some PIs mentioned. The RSC must come up with a strategy to address this, which may require additional financial support.

2. The research programs and the collaborative activities inside and outside RIKEN that are currently being conducted or are planned for the RSC (from the viewpoints of both scientific and societal impacts)

(Life Sciences)

Structural biology is certainly one of the RSC's main research activities. The RSC has played a key role in providing cutting-edge SR beamline technologies to the SPring-8 user community. The RSC's structural biology research has made a strong impact in the world scientific community, both in high throughput structural genomics and structural biology of membrane protein complexes. The related high-resolution structural information is important for biological as well as medical sciences but is still usually difficult to obtain. The RSC's own research activities in structural biology are also showing impressive progress and remarkable achievements in those two aspects as well. It is also important to note that the RSC has a few groups using electron microscopy (EM) and image analysis to study three-dimensional structures of large macromolecular complexes, membrane proteins and cells. Since EM is a complementary technique to X-ray diffraction, many of the EM image analysis techniques will be beneficial for single-particle diffraction imaging by XFEL. Thus the EM groups are expected to play important roles in research activities of the RSC as a whole.

However it is rather a shame that the RSAC members had an impression that the interactions between groups involved in structural biology should be better coordinated, as among the research teams in material sciences under the strong leadership of Dr. Takata. More cohesive interaction among groups in structural biology could be promoted by sharing more facilities and resources or by appointing some leading figure to review and coordinate the groups' activities.

The recent publication in Nature of the F-actin structure by X-ray fiber diffraction analysis was particularly impressive, not only because of the great scientific impact of the work but also because the RSC has maintained its support to this rather long-term study. This research required a unique superconducting magnet to make highly-oriented liquid-crystalline sol specimens of the F-actin filament and a specific beamline setup appropriate for high-quality fiber diffraction data collection. The study took more than a decade for Dr. Oda to complete. We expect the RSC to maintain support for such long-term, high-risk research activities.

(Materials Sciences)

Materials science is the RSC's other major research area on the SPring-8 campus utilizing accelerator-based light sources. RSC scientists rank among the world leaders in this area. The RSC has responded to recommendations from RSAC-2006 with specific developments. In particular, the establishment of the materials dynamics laboratory headed by Dr. A. Baron and the Structural Materials Science laboratory headed by Dr. M. Takata will keep the research of the RSC's materials team at the forefront.

The Materials Dynamics laboratory recently obtained funding for the development of a second beamline for inelastic X-ray scattering. This beamline, which will be the world's best for the foreseeable future, will open new research opportunities. Already the research of the laboratory has had important impacts on our understanding of the dynamics of novel superconductors ranging from insights in the 'classic' high TC systems to MgB2 to the recent Fe-As compounds. Most importantly, research teams have recently begun to investigate electronic excitations in the eV energy loss regime with meV resolution.

The advances in Takata's laboratory in the use of maximum entropy methods have been similarly impressive. They have recently moved from fitting the precise charge density and then deriving the electrostatic potential

to directly fitting the electrostatic potential. This is a very important step. These techniques have been applied to a wide variety of materials ranging from charge order in the manganites (important as GMR systems) to organic systems that show classic metal-insulator transitions

The RSC has been at the forefront of the manipulation of X-ray polarization and its use for both magnetic and chiral systems. The RSC is promoting research efforts in polymers and soft matter, and is generally maintaining a leading position. In this regard the RSC has established the quantum order research group with three sub-groups: spin order, spatial order and excitation order. Each group has generated promising results and the combination of research among the groups may be formidable.

Overall the RSC's materials research is very strong and well integrated in both the Japanese and the worldwide materials research communities. Of particular note is the outreach to the industrial community and the corresponding impact of the research. An exciting example is the study of the amorphous-to-crystalline transformation underlying the recording process for DVDs. This technique utilizes a unique combination of X-ray optics and science capabilities applied to an important technological area.

Also noteworthy is the construction and management of the RCS material science beamlines, which takes into consideration the entire beamline layout at the SPring-8 facility, where JAEA, NIMS and other institutions are developing their work on materials science.

3. The roles that the RSC is expected to take in the research complex (with JASRI and the XFEL) at the SPring-8 site.

The RSC focused on fulfilling the following responsibilities: 1) to support the activities of JASRI and 2) to play a leading role in the design and construction of the XFEL. The RSC plans to continue to fulfill these responsibilities for future development of the SPring-8 site. There is no doubt that the responsibility of the Riken Harima Institute, most naturally the RSC, will expand significantly once construction of the XFEL is completed. To maintain its internationally recognized level of excellence, the RSC will need more resources for both research and technical staff as well as additional budget for equipment and supplies. It is important for RIKEN to consider appropriate plans to support this crucial expanded role.

Recommendations

XFEL Research

The XFEL is expected to begin user operations two years from now. The RSC has enjoyed great success in carrying out world-class research at the SPring-8 facility. This research role has benefited and will continue to benefit the broad user community.

We recommend that a similar world-leading science program for the use of the XFEL be started within the Riken Harima Institute. This could potentially be accomplished by expanding the RSC. This expanded role would take best advantage of the existing expertise and technical developments.

Innovative Light Sources Division

The innovative light source division "gave birth" to the compact X-ray Free Electron Laser concept and the use of a pulsed DC electron gun. This division needs to play a key role in further development of the SPring-8 XFEL. The "SPring-8 II" initiative is now underway to upgrade SPring-8's synchrotron source. Note that the new chief scientist in this division will be in the general area of accelerator physics.

We recommend that this individual take a leading role in meeting the published goal of making SPring-8 II the "ultimate storage ring".

Photon Science Research Division

1) Life Sciences

The research of the individual teams in this area is of the highest quality. The teams include approximately

thirty scientists and ten postdoctoral researchers. The complementary expertise of the individual teams gives the RSC the potential to become a definitive internationally leading center in life sciences.

We recommend the appointment of a Life Sciences Coordinator to realize this potential. This role should help to:

1. Promote closer interactions among the research teams.
2. Ensure the continued development and optimal use of the research infrastructure and resources.

This coordinator position could be rotated among life science researches to take advantage of their various areas of expertise.

2) Materials Science

Energy and the Environment: The Noyori Initiative 4: RIKEN that provides international leadership in research.

We recommend that the RSC materials science teams investigate research opportunities related to energy and the environment with a focused, cross-cutting approach.
The RSC material science group should strive to be the world-leading center in this field by more collaboration with other groups in SPring-8 such as JAEA and NIMS.

New Initiatives

The Noyori Initiative 5: RIKEN that contributes to culture. The world synchrotron radiation community has begun to demonstrate progress using SR techniques as analytical tools for the study of cultural heritage artifacts and archeological finds.
We recommend that the RSC further explore these opportunities using Spring-8 facilities.

Advanced Photon Technology Division

Projects currently seem to emphasize the life sciences. We see a need at the photon technology division for life sciences and material sciences to be on an equal footing, as with the photon science research. This would inevitably lead to synergies that would benefit both areas. This need will be even greater when the XFEL begins operations and the requirement for advanced instrumentation to fully exploit the unique source properties becomes paramount.
This division should be strengthened and re-organized to meet these challenges.

Young Researchers

Young researchers are critical to the research environment and can make a significant impact at the RSC.
We recommend that the RSC look for initiatives to increase the engagement of young scientists in research activities.

Budget

With the recommended expanded role of the Harima Institute in the science program on the SPring-8 campus, any efforts that lead to increased resources are crucial to ensure the successful launch of the XFEL science program

2. Response to the Report

The RIKEN SPring-8 Center (RSC) greatly appreciates the reviewers' clear assessments of our scientific achievements during the three years following the RIKEN SPring-8 Center Advisory Council (RSAC) 2009 as well as the reviewers' careful recommendations concerning our future direction. We thoroughly studied the '**Recommendations of the RSAC-2009**', which was published in May 2009. We responded with the following opinions and comments:

The Director of the RSC, Dr. Tetsuya Ishikawa, greatly appreciates the positive evaluations of our challenging reorganization in response to the RSAC-2006 recommendations. Further reinforcement of the organization will be conducted with a view to the XFEL project completion and utilization commencement inside and outside of the RSC.

The Innovative Light Sources Division at RSC appreciates the committee's encouraging evaluation and recommendations. After the RSAC-2009 meeting, we started discussion about a grand design encompassing all surveys and research of XFEL science from the viewpoints of the feature of the second-generation IPs organization, XFEL user community commitment, etc. The specification of the Chief Scientist candidate was discussed after Dr. Kitamura's retirement. The new Chief Scientist should head a new laboratory developing technologies to make the best use of SPring-8 and XFEL for users including industrial sectors and also should lead the long-term project, "SPring-8 II 2019" and accomplish its objectives.

The Photon Science Research Division appreciates the suggestions regarding the coordination of research teams in the division, especially for Life Sciences. In fact, the excessive specialization and subdivision for the research activities of the structure biology groups resulted in the individual-oriented management of the laboratory. The division should start discussion about the strategies for coordination of laboratories to serve the facility mission including the promotion of a coordinator based on the recommendations. However, please note that RIKEN now has strict restrictions regarding the number of permanent positions. Therefore, career development and promotion encouragement for candidates both inside and outside the RSC should be structured to stimulate laboratory interactions toward the second phase of the RSC, for both the SPring-8 and XFEL facilities. For the first step, cross-cutting reviews of laboratories will be considered.
The materials groups appreciate the positive comments regarding the development of a cooperative research organization with leading scientists from organizations around the world. The new Inelastic Scattering beamline promotion and the research of the Quantum Order Research group will diversify the RSC's research network and promote the RSC as a the pivotal center for Photon Science. The Materials group will further explore research areas related to energy and the environment according to the recommendations.

The Advanced Photon Technology Division appreciates the committee's constructive suggestions for the enhancement of organizational channels to address science areas relating to the RIKEN beamlines as well as the entire SPring-8 and XFEL facilities. The division will develop the team organization to manage both the RIKEN beam lines and XFEL beam lines.

The RSC is on the way to reinforce the mission-oriented research organization to enhance the performance of the SR and XFEL facilities. The recommendations by the Advisory Council will become a lodestar in order to facilitate the evolution toward becoming the Leading Photon Science Research Complex featuring SPring-8 and XFEL.