1. Watching DVDs in Real Time

Digital versatile discs (DVDs) are one of the most convenient ways of storing large amounts of information. However, despite two decades of development since the discovery of the materials on which they are based, details of how they work remain unclear. Researchers from RIKEN SPring-8 Center, JASRI, CREST and Matsushita Electric Industrial are filling the gaps in our understanding of these materials, using state-of-the-art time-resolved X-ray diffraction analysis to observe the change in the atomic level structure of these materials.

This is a report on the first successful outcome of time-resolved pump and probe X-ray diffraction in SPring-8 by the pilot project "*X-ray pinpoint structural measurement*" organized by Japan Science and Technology Agency (JST) as the Core Research for Evolutional Science and Technology (CREST) started since 2004 and to be completed by 2009. The *X-ray pinpoint structural measurement* system is developed at the BL40XU high flux beamline (Fig. 1). The aim of the project is to achieve a picosecond time-resolved X-ray diffraction experiment using a submicron-scale beam. This is why the project is called "pinpoint." The aimed specifications of the X-ray pinpoint structural measurement are ~100 nm spatial resolution and ~40 ps time resolution. Specialists in the field of accelerator science, laser physics, X-ray optics, diffraction physics, crystallography and chemistry are part of this project (Fig. 2).

The research group has combined high-speed X-ray diffraction with *in situ* time-resolved laser reflectometry to simultaneously probe the structural and optical properties of two different DVD materials, $Ge_2Sb_2Te_5$ (GST) and $Ag_{3.5}In_{3.8}Sb_{75.0}Te_{17.7}$ (AIST). This has enabled them to track microscopic processes that occur in these materials, in real-time, as they change from an amorphous state to a crystalline state. They found a gradual increase in both the reflectivity and emergence of diffraction peaks corresponding to the crystalline phase, proving the close relationship between the optical properties and structures of the materials. The differences in the widths of the diffraction peaks between the two materials and their evolution over time led the researchers to propose two subtly different models of the mechanisms taking place in each. In GST, they suggested that large crystal grains form over the entire volume of the material when the moment the process starts; however, in AIST, the process begins with the formation of small crystallites in different parts of the material, which gradually grow and merge to form

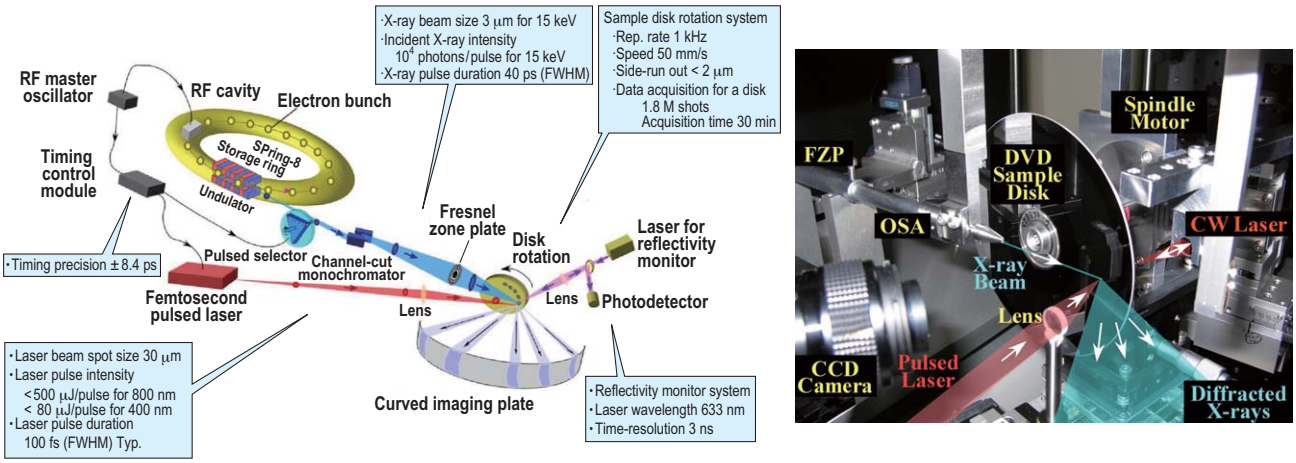

Fig. 1. Schematic representation and photograph of *X-ray pinpoint structural measurement system.*

larger grains. The level of detail enabled by this and future studies is likely to make a valuable contribution to the development of better and faster DVD materials.

The X-ray pinpoint structural measurement system is now close to completion in SPring-8. The system, which is an integration of a time-resolved experiment and a sub-micron beam technique, will be applied after its completion to the study of various phenomena such as photo-induced phenomena, and structural changes under applied AC electric field.

Fig. 2. Members of *X-ray pinpoint structural measurement project.*

2. Capturing a Heartbeat Motion

Internal motions such as heartbeat, and the pulsation of blood vessels, are inherent in all living creatures. In a hospital, we are told to hold our breath when chest X-ray or CT images are taken to avoid motion blur. However, it is impossible to control heartbeat. A research team composed of researchers from RIKEN, Kawasaki University of Medical Welfare and JASRI has designed and constructed a high-resolution, computed tomography (CT) system that can sharply visualize the motion and deformation of the heart, coronary arteries and small airways of live mice and rats, which are most often used as animal models of human diseases.

Mice and rats have heart and respiration rates higher than 300 and 100 per minute, respectively, making internal motions very fast. Since these animals are smaller than humans, the required spatial resolution is higher, making motion blur a more serious problem.

The RIKEN team solved this problem by controlling respiration with a ventilator and monitoring heartbeat using an electrocardiogram. Using a fast X-ray shutter, images were recorded only when the respiration and heartbeat were in their certain prescribed phases. By rotating the animal in the X-ray beam and collecting images, the team was able to accumulate data for the 3D reconstruction of the chest. For more details on this topic, see page 50 of this issue.

Figure 3 shows a comparison of the reconstructed cross sections of a mouse chest. The resolution is 12 μm per pixel. The left image (A) is without synchronization, showing severe blurring. The center image (B) is with only respiration synchronization, showing blurring of the heart. The right image (C) is with respiratory and cardiac

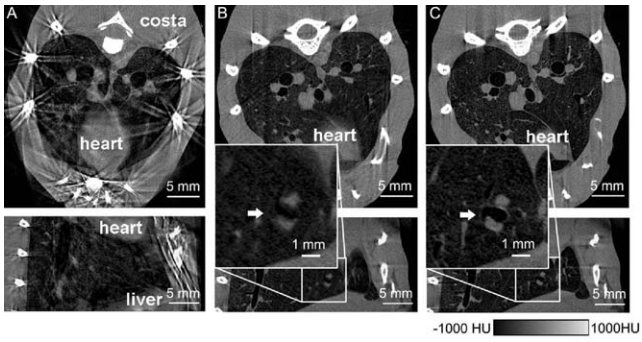

Fig. 3. Reconstructed cross-sections of mouse chest by high-resolution computed tomography (CT).

synchronizations. The blurring is much reduced and the bronchi and the heart are clearly visualized. Using this technique, they constructed sharp images of the lung after inspiration and expiration, and also those of the heart in systole and diastole.

This technique opens a way to high resolution imaging studies of live animals. The high-resolution dynamic structures of the lung and heart will help in our understanding of the function of these vital organs, especially by providing an experimental basis for the simulation of gas exchange in small airways and of shear stress in blood vessels using a supercomputer.

3. Coming Powerful Light

SPring-8 will soon start building a new beamline for inelastic X-ray scattering, i.e., the Quantum Nano Dynamics Beamline BL43LXU, which has been funded by MEXT through RIKEN. The new beamline will provide unprecedented flux using a short-period, small-gap undulator installed in one of SPring-8's 30-m straight sections. By operating in the fundamental to maximize the ratio of flux to power load, such a flux will be the world's most brilliant X-ray source in the 15 to 25 keV energy range, and provide the highest flux, as shown in Fig. 4.

Associate chief scientist Alfred Baron has been considering this project for more than 4 years and has a numerous discussions with scientists about the scientific goals for such a beamline - the members of the workshop in 2008 are shown (Fig. 5). The beamline's scientific target, i.e., inelastic X-ray scattering with energy resolutions from <1 to >40 meV covers some of the most challenging experimental regimes today: the high-resolution (1 to 3 meV) setup is aimed primarily at atomic dynamics in crystals and disordered materials, and the “medium-resolution” (6 to 40 meV) setup at nonresonant measurements of charge dynamics. This

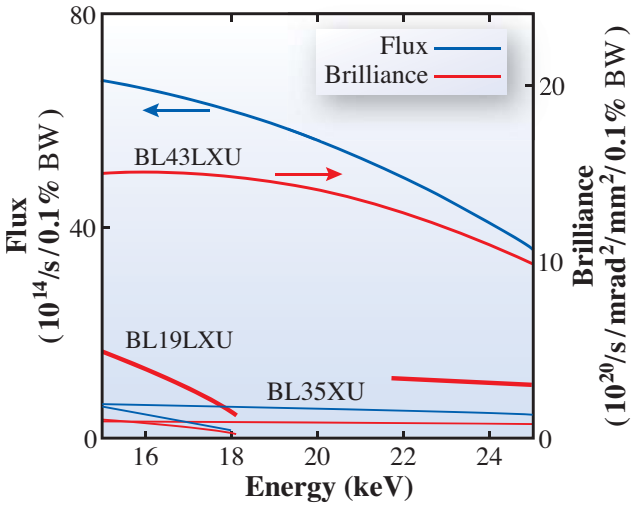

Fig. 4. Comparison of the flux and brilliance available from a standard insertion device (32 mm period by 4.5 m long) at BL35XU and the one planned for BL43LXU (19.4 mm period, 17.6 m). The brilliance of BL19LXU (32 mm period, 25 m) is included for reference.

is expected to provide a unique window on processes in many different types of material, and in different potentially extreme conditions. One area of application, for example, will be in the new iron-arsenic superconductors discovered by Hosono's group. With superconducting transition temperatures that are only exceeded by those of some copper oxides, this new class of high-temperature superconductors shows a complex electronic structure, magnetic order, and an extremely strong magneto-elastic coupling. The twin windows of meV resolution for investigating atomic dynamics and of ~40 meV resolution for investigating electronic dynamics are expected to lead to new results - in addition to the investigation of magneto-elastic interaction, for example, direct investigation of superconducting gap may be possible.

Fig. 5. Workshop for new beamline “Quantum Nano Dynamics Beamline.”

4. Heading to Next Goal: Sunbeam Consortium

In the last decade, the Sunbeam Consortium (Industrial Consortium for Beamline Construction and Applications) has contributed to new technology developments as the front runner in industrial utilization with the Industrial Consortium Beamline (BL16XU/B2). The Sunbeam Consortium is a private organization consisting of 13 companies (12 companies and 1 electric group): Kawasaki Heavy Industries, Ltd., Kobe Steel, Ltd., Sumitomo Electric Industries, Ltd., Sony Corp., Electric power group (Kansai Electric Power Co., Inc., Central Research Institute of Electric Power Industry), Toshiba Corp., Toyota Central R&D Labs., Inc., Nichia Corp., NEC Corp., Hitachi, Ltd., Fujitsu Laboratories Ltd., Panasonic Corp. and Mitsubishi Electric Corp.

The SPring-8 research of the Sunbeam Consortium has successfully been applied to the development and improvement of manufacturing processes for various types of product such as advanced semiconductor devices, high-density magnetic disks, laser diodes, optical fibers, high-corrosion-resistance steel, automotive catalysts and fuel batteries.

On the basis of the activities over the past 10 years and the next-term research plans, the Sunbeam Consortium renewed their contract with JASRI, who is in charge of SPring-8 operation, for the continuous installation and operation of the Industrial Consortium Beamline for the next 10 years starting from August 27th, 2008.

For the next term, a large-scale capital investment of approximately 320 million yen was made to renew the experimental equipment (Fig. 6). The main upgrades achieved are as follows:

(i) *X-ray diffractometer and scattering measurement system*

The system increased the number of movable axes of the sample stage from 4 to 8. This improvement can provide high measurement flexibility and reduce measurement time to half. The new large sample stage allows the mounting of a large wafer up to 300 mm diameter and the measurement of the entire product, instead of a test piece or a cut-out sample.

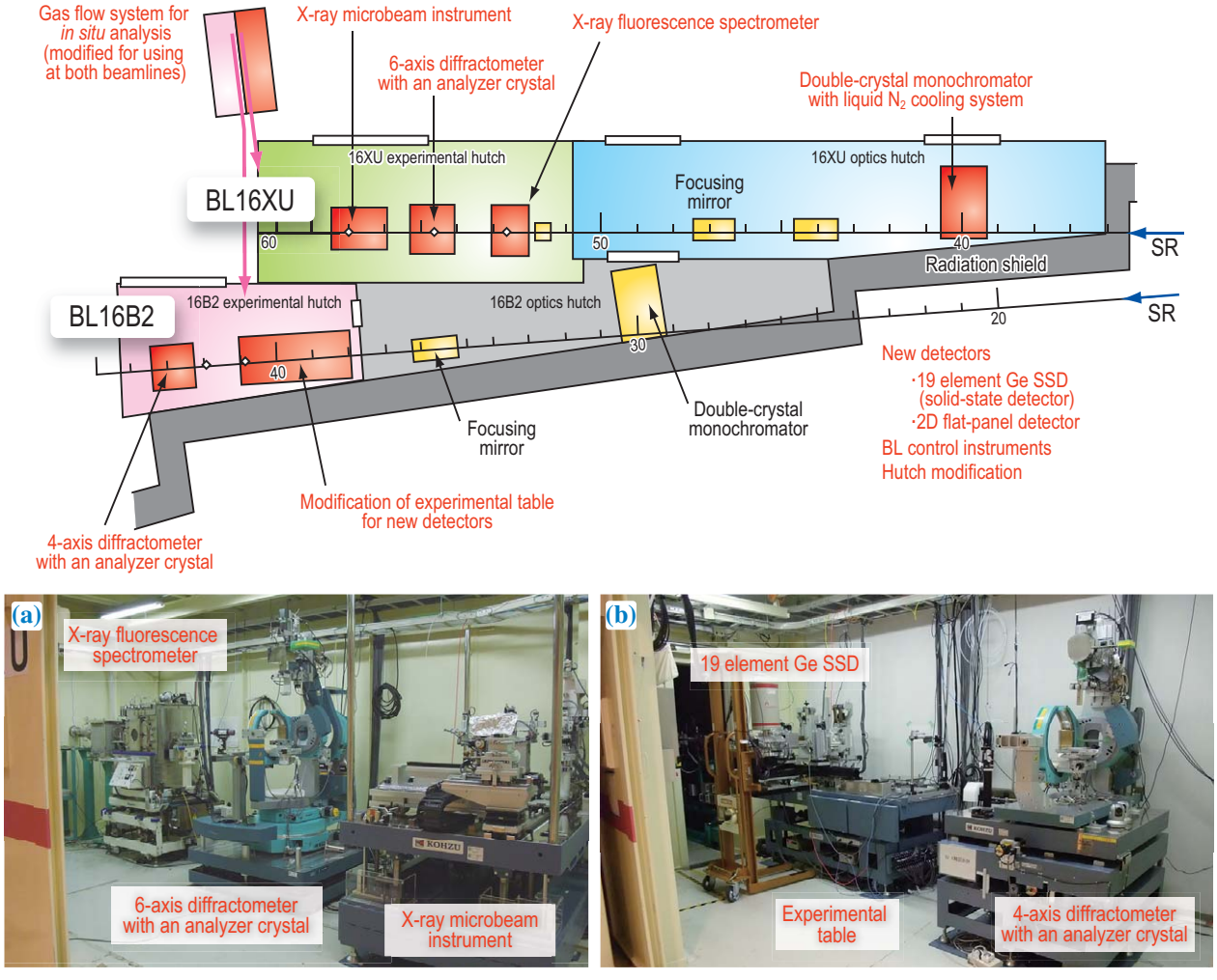

Fig. 6. Beamline diagram and photograph of the Industrial Consortium Beamline **(a)** BL16XU and **(b)** BL16B2. Upgraded parts of experimental equipment are indicated in red.

Consequently, the structure and interface structural analysis of a 1-nm silicon oxide layer on a 300-mm-diameter wafer used in the production line has been accomplished; it is the world's highest precision measurement. This achievement is also made possible by significant progress in the dynamic range of measureable data up to 12 orders of X-ray intensity magnitude from 10 orders of magnitude for the X-ray reflectivity measurement.

(ii) *X-ray fluorescence measurement system*

The element analysis is available even for ultra-dilute samples. The element mapping area also increased to be applicable to 200-mm-diameter wafers with 10 μm resolution. Chemical state analysis is also available as well as composition analysis with XAFS measurement. High-performance equipment will provide a solution to the various types of problem concerning devices, and contribute to the development of novel sustainable materials and commercial products such as hexavalent-chromium-free plating.

(iii) *Microbeam technique*

The function of X-ray diffraction analysis is related to the focused beam whose diameter is less than 300 nm. X-ray intensity increases over one order of magnitude at the sample position. This technique enables microstructure analysis, such as designing a micro-magnetic head for high capacity, analyzing head materials, and improving the fabrication process.

Full operation was restarted from the second half of the fiscal year 2008. The utilization of the new facilities and equipment will allow previously unattainable level of analyses and observations, such as ultrathin-film and sub-micrometer analysis, real-time observation and direct observation of commercial products.

5. Finding a Way to Overcome Diseases

From the beginning of modern drug discovery, any new drug is the result of complex efforts includes many steps such as assays, clinical trials and among others. Even today, drug development takes years, and the costs for screening and safety testing are very high and rising. Discovering drugs targeting infectious diseases has the added complication that a single mutation of the target virus or microbes may render the drug ineffective. Therefore, rapid drug discovery is even more important in this case; moreover, such drugs should target some essential biological process to limit survival of the pathogen.

Structure determination of drug-target proteins has long been recognized to assist drug discovery, because knowledge of the protein structure helps build drugs which fit into it and bind tightly. Recent developments in structural biology, including the improvement of synchrotron beamlines, have greatly accelerated the pace of protein structure determination, and enabled structural genomics groups to solve drug-target proteins very rapidly. Although the number of the results are not so much more but several important drugs has been developed.

For example, the influenza drugs zanamivir (Relenza) or oseltamivir (Tamiflu) target the viral neuraminidase, which is an essential protein for release of the virus from host cells. Unfortunately, influenza can develop resistance to these drugs, and new ones are urgently required to treat such resistant strains.

In 2008, Prof. Park and his group from Yokohama City University have determined the structure of a piece of the influenza RNA polymerase. This family of enzymes is essential to all biological species, being required to utilize genetic information stored in DNA. However, the influenza enzyme is assembled from three polypeptide chains unique to the virus, and disruption of its assembly blocks replication of the virus inside host cells. Two subunits, called PA and PB1, bind together through part of their structure to form a complex, which is necessary for the RNA polymerase to function. The structure of this complex revealed the interaction between subunits, and this structure is being used to guide new drug development (Fig. 7). Detail in this topic can be found in Park *et al.*'s report in this issue on page 18.

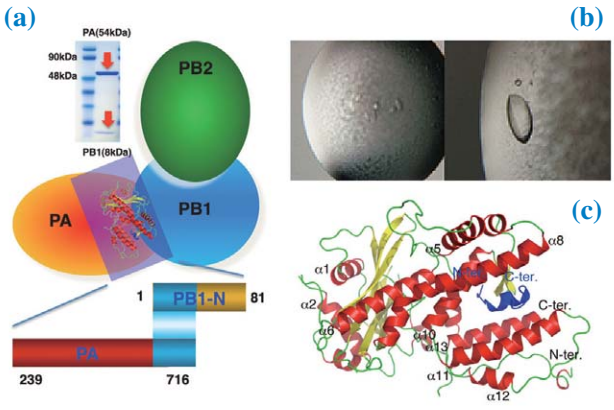

Fig. 7. Influenza RNA polymerase complex. **(a)** Schematic diagram of PA, PB1 and PB2 subunits of the influenza RNA polymerase. **(b)** Crystals of the complex. **(c)** An overall ribbon diagram showing the fold of PA, with helices in red, strands in yellow and coil in green. Helices are numbered from the N terminus. PB1 residues are in dark blue.

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