PF-AR NW14, A New Time-resolved Diffraction/Scattering Beamline

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Abstract. NW14 is a new insertion device beamline at the Photon Factory Advanced Ring (PF-AR), which is a unique ring with full-time single-bunched operation, aiming for time-resolved X-ray diffraction/scattering and XAFS experiments. The primary scientific goal of this beamline is to observe the ultrafast dynamics of condensed matter systems such as organic and inorganic crystals, biological systems and liquids triggered by optical pulses. With the large photon fluxes derived from the undulator, it should become possible to take a snapshot of an atomic-scale image of the electron density distribution. By combining a series of images it is possible to produce a movie of the photo-induced dynamics with 50-ps resolution. The construction of the beamline is being funded by the ERATO Koshihara Non-equilibrium Dynamics Project of the Japan Science and Technology Agency (JST), and the beamline will be operational from autumn 2005.

1. Introduction
Molecular dynamic imaging, which gives time-resolved images of precise atomic motion, is a very important technique \cite{1,2} in dynamics studies of chemical or biological systems and condensed matters. AR-NW14 is a new insertion device beamline at the PF-AR designed for time-resolved X-ray diffraction/scattering and XAFS studies of condensed matter samples such as organic \cite{3,4} and inorganic materials \cite{5-7}, protein crystals \cite{8,9} and liquids \cite{10-12}. PF-AR at the High Energy Accelerator Research Organization (KEK), Tsukuba, Japan is a full-time single-bunch synchrotron radiation source operated for such time-resolved X-ray studies using pulsed X-rays. By utilizing the full advantage of the sparse bunch structure of the PF-AR ring, we aim to develop sub-nanosecond-resolved X-ray structural analysis capabilities. The primary scientific targets of the AR-NW14 will be condensed matter systems which can be triggered reversibly by a laser pulse. In particular, photo-induced phase transitions (PIPT) in molecular charge-transfer (CT) crystals are one of the main...
candidates for our research. The remarkable feature of PIPT is its cooperativity, that is, the structural relaxation of the electronic excited state of a molecule causes a large-scale photo-induced phase transformation towards a new lattice, electronic order and physical properties. Time-resolved X-ray diffraction enables direct access to the dynamics of electronic, atomic and molecular motions in such systems. In principle, one can construct 50-psec still images of the electron density at a given delay after initiation and produce a "movie" of the reaction with atomic resolution. The relative delay time between the laser and X-ray pulse is controlled by an electronic delay generator based on the radio frequency master clock (508 MHz) that drives the electron bunches in the storage ring.

2. X-ray source
The beamline has two undulators with period length of 36 mm (U36) and 20 mm (U20). The brilliance of U36 and U20 are shown in figure 1. The U36 covers an energy range of 5-25 keV with 1st, 3rd, and 5th harmonics, which is used as a tunable and intense monochromatic X-ray source by using a double-crystal monochromator and a focusing mirror. The typical photon flux of the monochromatic beam is estimated as $\sim 10^{15}$ photons/sec. The U20 gives the 1st harmonic in the energy range of 13-20 keV. The energy bandwidth of the 1st harmonic is $\Delta E/E \sim 10^{-2}-10^{-1}$, which can be utilized as ‘narrow-bandwidth white beam’ or ‘wide-bandwidth monochromatic beam’ with photon flux of $\sim 10^{15}$ photons/sec. With these photon fluxes, it should become possible to take a snapshot an atomic-scale image of electron density distribution. The X-ray pulses are delivered at a frequency of 794 kHz with the pulse duration of $\sim 50$ ps (rms). The focused beam size at the sample position will be 0.2 mm (V) x 0.6 mm (H).

Figure 1. The brilliance of U36 and U20.

3. Overview of Beamline
A plan view of the beamline and a virtual image of the Optic and Experimental hutches are shown in figure 2 and 3. The front end consists of a fixed mask, a beam-position monitor, an absorber, a beam
Figure 2. A plan view of the beamline.

shutter, a graphite heat absorber, XY-slits for white X-rays and Be windows. The main optical components are a double-crystal monochromator and X-ray mirror system, which are located 30.5 m and 39-42 m from the center of insertion device U20, respectively. The double-crystal monochromator consists of flat Si(111) crystals, which are cooled with liquid nitrogen in order to reduce any deformation caused by the heat loads. The cooling system can handle an incoming heat load of up to 450 W. The X-ray mirror system has 3 mirror assemblies: a bent cylindrical mirror for focusing of X-rays, and a double-mirror system (cut-off mirrors) to reduce a contamination of the higher harmonics.

Figure 3. A virtual image of the Optic and Experimental hutches.
4. X-ray pulse selector
In order to collect diffraction/scattering images with 2-dimensional detectors such as CCDs or imaging plates, we need to use a chopper to synchronize the X-ray and laser pulses in a 1:1 ratio, since the available detectors presently have no gating capabilities. A high speed chopper (X-ray pulse selector, XPS) which is synchronized at 946 Hz to a subharmomic (1/537600) of the radio frequency and made by Forschungszentrum Jülich can be used for this purpose. The XPS is shown in figure 4. The physical opening window of the chopper corresponds to 1.2 µsec but when it is phased to select the single bunch in the PF-AR single bunch mode, the exposure time becomes the 50 psec duration of the X-ray pulse. The novel feature of the chopper is its continuous phase locking with a timing jitter of less than 2 nanoseconds. One can thus produce a 946 Hz pulse train of 50 psec pulses from the X-ray pulse trains at 794 kHz emitted from PF-AR ring. If a detector with gating capabilities such as an avalanche photodiode is used, the XPS is not needed, and a gated integrator system can be used instead. If the repetition rate of the reversible reaction is slower than 946 Hz, a millisecond single-shot shutter will be available to lower the repetition rate.

![X-ray pulse selector](image)

**Figure 4.** X-ray pulse selector made by Forschungszentrum Jülich.

5. Diffractometer
NW14 has three diffractometers: Huber 7-axis, Rigaku cylindrical imaging plate, and Rigaku Mercury CCD. These diffractometers are shown in figure 5. Sample crystal can be cooled down to 10 K by using cryogenic helium gas flow (Rigaku, XR-HR10K) and the closed cycle He cryostat in the Be dome on the Huber 7-axis diffractometer.

6. Femtosecond laser system
A double pulse train of exciting laser pulses followed by probing X-ray pulses can be produced in which the relative delay time can be varied by the use of an optical delay line. A Ti:sapphire regenerative amplifier laser system will be operated, to produce exciting light pulses up to 800 µJ/pulse at 800 nm at a repetition rate of 946 Hz. The seeding laser is operated at 1/6 of the radio
frequency of the master clock (508 MHz) that drives electron bunches in the storage ring to synchronize with the X-ray pulses. Synchronization between the laser and the X-ray pulses is achieved by dynamically controlling the cavity length of the seeding laser. This 1/6 frequency divider is used for the coarse control of the relative delay with 2-ns resolution. The fine control of the relative timing is achieved by an optical delay line up to ~3 ns. An optical parametric amplifier will also be installed, to cover wider spectral regions from visible to mid-infrared.

Figure 5. The three diffractometers equipped in NW 14: (a) Huber 7-axis, (b) Rigaku cylindrical imaging plate, and (c) Rigaku Mercury CCD.

7. Schedule for the construction
The construction of the beamline is being funded by the ERATO Koshihara Non-equilibrium Dynamics Project of the Japan Science and Technology Agency (JST), and this beamline is planned to be fully operational from autumn 2005.

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