

BL12XU NSRRC ID

1. Introduction

BL12XU is one of the two contract beamlines operated by the National Synchrotron Radiation Research Center (NSRRC), Taiwan. It is designed mainly to support inelastic X-ray scattering (IXS) experiments and hard X-ray photoemission spectroscopy (HAXPES). BL12XU has an undulator light source and two branches, namely, the mainline and sideline (Fig. 1). The mainline, which has been fully operational since 2001, is used by both domestic and international scientists for IXS. The sideline is used for HAXPES. The HAXPES end-station is open to general users, although some adjustments and upgrades by the Max-Planck Institute for Chemical Physics of Solids (MPI-CPfS) are ongoing.

In June 2020, NSRRC and RIKEN/JASRI agreed on the extension of the contract for the 12XU and B2 operations for further six years. The two beamlines are expected to be used in the exploration of science and industrial applications in the high-energy region, where Taiwan's Photon Source is less effective.

2. Instrumentation

On the basis of "Future Plan" submitted to JASRI/RIKEN prior to the contract extension, the upgrading of the beamline and end-stations is in progress. Two examples are briefly introduced below.

RIXS analyzer revolver: X-ray absorption spectroscopy (XAS) based on high-energy-resolution fluorescence detection (HERFD) is a kind of resonant inelastic X-ray scattering (RIXS). The incident photon energy is scanned across an absorption edge by monitoring the peak intensity of an emission line at a high resolution (e.g., 1 eV). The advantage of HERFD-XAS is the suppression of lifetime broadening on XAS spectra. Nevertheless, the energy range covered by the spherical analyzer used in this technique is rather narrow, and thus, it must be changed, which would require an alignment each time if one tries to measure other elements or edges. This fact limits the speed of data acquisition. To overcome this limit, we have developed an analyzer revolver, which can

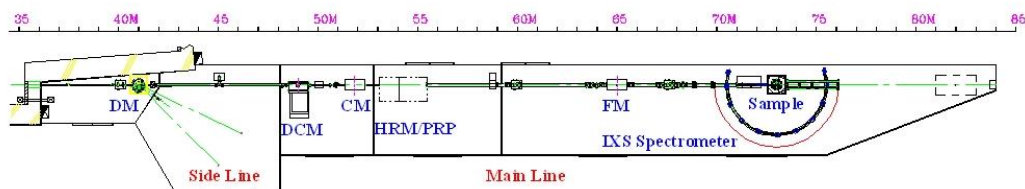


Fig. 1. Schematic diagram (top view) of BL12XU: DM is a diamond monochromator for the sideline, DCM a double crystal monochromator for the mainline, CM a collimating mirror, HRM a high-resolution (channel cut) monochromator, PRP a phase retarding plate, FM a focusing mirror, and IXS an inelastic X-ray scattering spectrometer.

accommodate a maximum of four analyzers (see Fig. 2). It allows users to switch the analyzer by remotely rotating the revolver. The rotation is reproducible and the alignment is automated, so that the users can switch the analyzers with a simple command any time they wish.

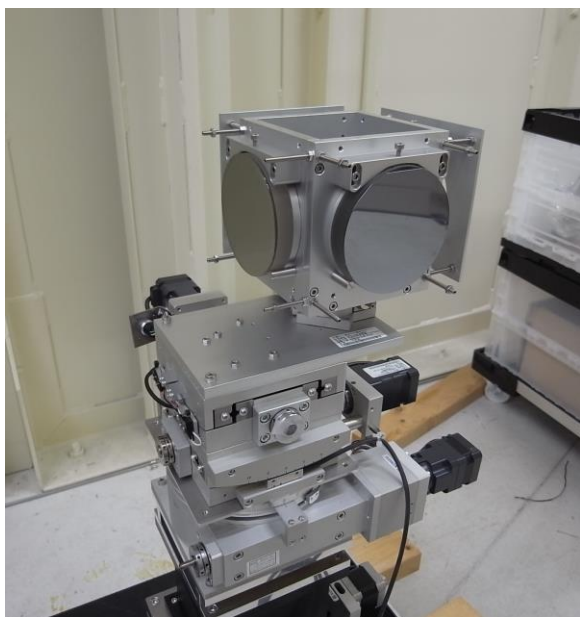


Fig. 2. Analyzer revolver developed for HERFD-XAS.

Multi-arm Laue spectrometer: We developed a Laue spectrometer in the past decade to enable experiments in an energy range above 20 keV. We are now attempting a major upgrade of this spectrometer. Presently, it has a single arm consisting of a triangular analyzer and a NaI detector. We are currently preparing five arms to increase the count rate (see Fig. 3). In FY2020, we designed, drew up, and purchased essential components such as analyzer crystals, benders, detectors, and their stages. In FY2021, we will assemble and test them. Once this upgrade is completed, we will be able to carry out various applications, for example, IXS studies across the Li K-edge on lithium batteries, the C or O K-edge on

super/subcritical solvents, and the Mg, C, Be, or other absorption edges of low-Z element additives in Al, Fe, or Cu alloys.

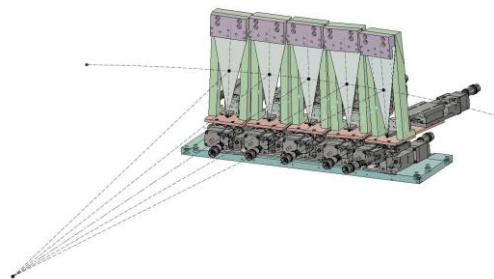


Fig. 3. Schematic of analyzers in the multi-arm Laue spectrometer.

3. Experiments

In FY2020, because international and domestic travel was strictly limited as a result of the worldwide COVID-19 pandemic, most of the external user experiments were cancelled. Therefore, the available beamtime was used to upgrade the beamline and end-station or to test remote experiments with overseas users. Both tasks were well accomplished and significant progress was achieved. Regarding publications, 20 papers and two Ph.D. theses were produced as a result of using 12XU. They include six papers for HERFD-XAS studies on 3d/4f correlated electrons [1-6], six for studies on catalysts [7-12], two for nonresonant IXS studies on gas or liquid [13,14], two for HAXPES studies on 3d/5d correlated electrons [15,16], and four for others, e.g., high-resolution Compton scattering studies [17,18]. Representative papers are briefly introduced below.

Concomitant singularities of Yb-valence and magnetism at a critical lattice parameter of icosahedral quasicrystals and approximants: Quasi-crystals (QCs) are metallic alloys that

possess a long-range quasiperiodic structure with a specific type of diffraction symmetry, such as five- or tenfold rotational symmetry, which is incompatible with translational symmetry and hence forbidden to periodic crystals. An approximant crystal (AC) is a periodic phase with a composition close to that of a QC. Imura and co-workers determined the valence numbers of Yb ions in QCs and ACs by HERFD-XAS. They found that Yb ions exhibit a fluctuation between 2+ and 3+, but there is a critical lattice parameter where Yb-valence and magnetism concomitantly exhibit singularities [4].

Charge-transfer energy in iridates: A hard X-ray photoelectron spectroscopy study: The class of iridium oxide materials has recently been attracting broad interest owing to the expectation of exotic magnetic states. Takegami and co-workers investigated the electronic structure of iridates in the double perovskite crystal structure containing either Ir⁴⁺ or Ir⁵⁺ using HAXPES. The experimental valence band spectra could be well reproduced using tight-binding calculations including only the Ir 5d, O 2p, and O 2s orbitals. They found that, regardless of the A and B cations, A₂BIrO₆ iridates have essentially zero O 2p to Ir 5d charge-transfer energies, indicating that double perovskite iridates are extremely covalent systems [15].

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