

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: 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 opened 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 explore science and industrial applications in the high-energy region, where Taiwan 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 the end-stations are running. The two major instruments that are being upgraded are (i) an analyzer revolver for the resonant inelastic scattering spectrometer and (ii) a multi-arm Laue spectrometer for a nonresonant inelastic scattering spectrometer. In 2020, the analyzer revolver was installed, and the commissioning was successfully completed. In 2021, efforts were focused on the construction of the multi-analyzer-detector arms for the Laue spectrometer.

Multi-arm Laue Spectrometer: In the past decade, we developed a Laue spectrometer to activate experiments in an energy range above 20 keV. We are now attempting a major upgrade on this spectrometer. Presently, it has a single arm consisting of a bent crystal analyzer and a NaI detector. We are adding four arms to increase the count rate (Fig. 2). In FY2020, we designed, drew

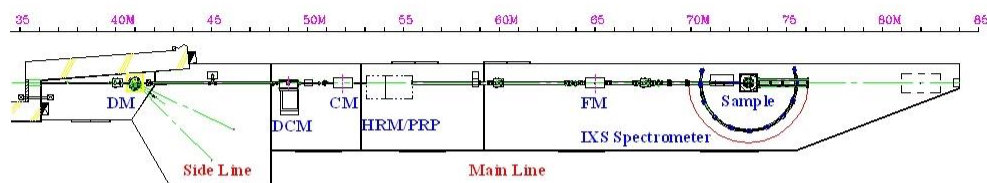


Fig. 1. Schematic diagram (top view) of BL12XU: DM is a diamond monochromator for the sideline, DCM a double crystal monochromator for the mainline, CM a collimating mirror, HRM a high-resolution (channel-cut) monochromator, PRP a phase-retarding plate, FM a focusing mirror, and IXS an inelastic X-ray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

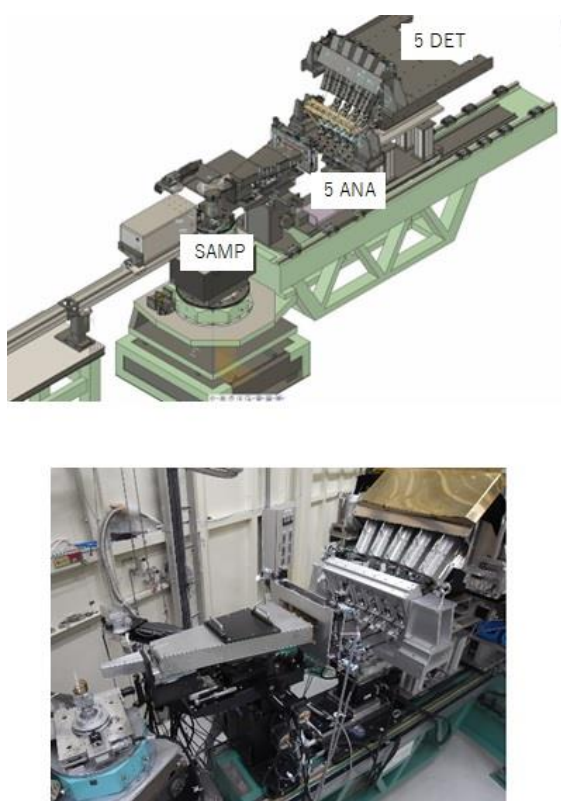


Fig. 2. Drawing and photo of multi-arm Laue spectrometer

up, and purchased essential components such as analyzer crystals, benders, detectors, and their stages. In FY2021, we assembled and tested them. An error in the design was found during the commissioning. We calculated the analyzer angles and detector positions at the limit of the zero Bragg angle, $\theta_B \rightarrow 0^\circ$. It was assumed that the deviations would not be so large even at a finite θ_B , e.g., $\theta_B = 30^\circ$. This assumption is not correct. The deviations crucially affect the positions and angles of the beam reflected by the analyzers. Because of this fact, the two outsides of the five detectors provided much lower intensities and energy resolutions than the others inside. In 2022, we will attempt a recommissioning after fixing the problems.

3. Experiments

In FY2021, the restriction of international travel continued, and thus most of the user experiments were cancelled except for those by Japanese users. The available beamtimes were used for upgrading the beamline and end-station or tests for remote experiments with overseas users. Both tasks were well managed. Regarding publications, 16 papers involving BL12XU were published. They include six papers on high-energy-resolution fluorescence detection (HERFD-) XAS studies on 3d/4f strongly correlated electron systems^[1-6], four papers on catalysts^[7-10], one paper on nonresonant IXS studies on liquids^[11], and five papers on HAXPES studies on 3d/5d correlated electrons^[12-16]. Representative papers are briefly introduced below.

Double-atom Catalysts as a Molecular Platform for Heterogeneous Oxygen Evolution Electrocatalysis: HERFD-XAS is becoming an increasingly popular tool for studies on catalysts. Generally, the spectral resolution in XAS is limited by the lifetime broadening of a core hole. This fact makes it difficult to resolve small features near the main edge. However, one can suppress such a lifetime broadening in HERFD-XAS. Exploiting this advantage, Bai et al. revealed a chemical reaction in the synthesis of Co-, Fe-, and Ni-containing double-atom catalysts, which exhibit excellent performance in the oxygen evolution reaction^[10]. The initial material is a single-atom catalyst including transition metal (TM) atoms (e.g., Ni). When they are subjected to electrolysis in a commercial KOH solution that contains some amount of other TM (e.g., Fe), the OER activity is gradually enhanced. HERFD-XAS revealed how 3d TM ions in a single-atom catalyst are connected to other TM ions in the solution to become double-

atom electrolytes.

Electronic Structure of Metallic Oxide ReO_3 : Transition-metal oxides display a considerably wide range of fascinating physical phenomena. The oxide ReO_3 is atypical: it is nonmagnetic despite its d shell being partially filled, and it is highly metallic. In fact, it has the highest conductivity of all oxides, comparable to that of copper or silver. The temperature dependence of the resistivity is considerably strong and signals the important role of optical lattice vibrations. Falke et al. investigated the electronic structure of the metallic oxide ReO_3 by bulk-sensitive angle-resolved soft-X-ray and angle-integrated hard-X-ray photoelectron spectroscopy^[16]. They observed clear dispersions of the Re 5d and O 2p derived bands as well as the momentum splitting of the Fermi surface due to the Re 5d spin-orbit interaction. It was shown that the density-functional-based band structure methods can provide an accurate description of the observed electronic states with hybrid functionals.

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