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 the 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 has been open to general users since 2011. This end-station is co-operated with the Max-Planck Institute for Chemical Physics of Solids (MPI-CPfS), Germany.

In June 2020, NSRRC and RIKEN/JASRI agreed on the extension of the contract for the 12XU and B2 operations for a further six years. The two beamlines are expected to aid research in the high-energy region, where Taiwan Photon Source is less effective.

2. Instrumentation

The beamline major upgrading of 12XU and B2 will be performed in FY2023–2026. We are expected to complete the preparations for the so-called SPring-8-II project, that is, a ring upgrading to produce brilliant synchrotron radiation. In FY2022, we studied the monochromators, mirrors, and other optics for 12XU (and B2). The end-stations were also studied. In addition to the current end-stations for inelastic X-ray scattering and for the hard–X-ray photoemission spectroscopy, a new end-station for the coherent diffractive imaging will be built in the middle hutch in 12XU.

One of the main upgrading tasks in 12XU is a modification on the monochromator. Double

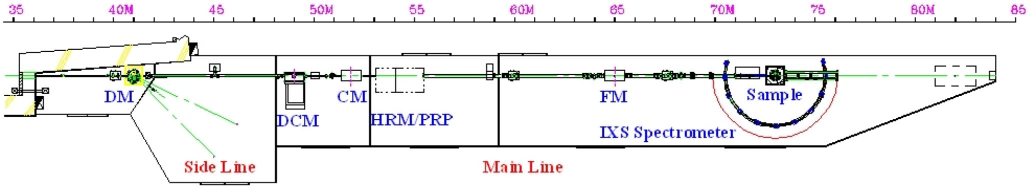

Fig. 1. Schematic diagram (top view) of BL12XU. DM is a diamond monochromator for the sideline, DCM a double-crystal monochromator for the mainline, CM a collimating mirror, HRM a high-resolution (channel cut) monochromator, PRP a phase retarding plate, FM a focusing mirror, and IXS an inelastic X-ray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

multilayer mirrors (DMM) will be installed so that a high-flux beam will be available. The estimated enhancement in flux is 5–20-fold compared with those by the Si111 current monochromator. In addition, Si220 crystals will be newly added in parallel to the Si111 crystals currently existing, so as to produce a higher energy (6–60 keV), narrower bandwidth ($dE/E=0.6\times10^{-4}$) beam with flux approximately half of those produced using Si111. Figure 2 shows the interior of the monochromator chamber of 12XU. The first multilayer mirror will be placed before the Si crystals while the second one after the Si crystals. The DMM works at the Bragg angle of around 1.48° and reflects the beam at ~11 keV and ~17 keV with multilayers of different periods. The monochromator will be installed with the Si double crystals in 2023 and reinstalled with the double multilayer mirrors in 2024 (or 2025).

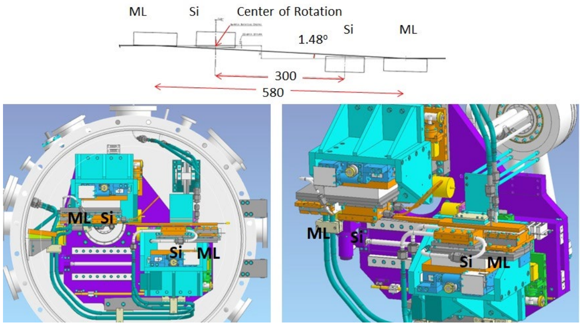

Fig. 2. Geometry of double-crystal/multilayer monochromator and the schematic presentation of the interior of the monochromator chamber.

3. Experiments

In FY2022, until October, the restriction on international travel remained in effect, and thus most of the experiments were performed by Japanese users. After the restriction was lifted, Taiwanese users returned to the beamline for their experiments. Regarding publications, 15 papers were produced from 12XU. They include six papers for high-energy-resolution fluorescence detection (HERFD-) XAS studies on 3d/4f strongly correlated electron systems [1-6], one for that on catalysts [7], and seven for HAXPES studies on 3d/5d correlated electrons [8-14] and one for that on semiconducting functional materials [15]. Representative papers are briefly introduced below.

Robustness of superconductivity to external pressure in high-entropy-alloy-type metal telluride AgInSnPbBiTe$_5$: High-entropy-alloy (HEA) superconductors are a new class of disordered superconductors. Mizuguchi and his team (Tokyo Metropolitan University) investigated the robustness of superconducting states in HEA-type metal telluride (MTe; M = Ag, In, Sn, Pb, Bi) under high pressure [1]. PbTe exhibits a structural transition from a NaCl-type to an orthorhombic Pnma structure at low pressures, and further transitions to a CsCl-type structure at high pressures. When the superconductivity of the CsCl-type PbTe is observed, it is found that its superconducting transition temperature (T_c) decreases with pressure. However, in the HEA-type AgInSnPbBiTe$_5$, T_c is almost independent of pressure at pressures ranging from 13.0 to 35.1 GPa. To clarify the effects of the modification of the configurational entropy of mixing on the crystal structure, superconducting states, and electronic structure of MTe, HERFD-XAS was performed at 12XU for three MTe polycrystalline samples of PbTe, $AgPbBiTe_3$, and $AgInSnPbBiTe_5$ with different configurational entropies of mixing at the M site.

Direct imaging of valence orbitals using hard X-ray photoelectron spectroscopy: One of the main applications and most widespread applications of HAXPES is the use of its deep probing depth to probe the real electronic structure to avoid effects from the surface, which may be contaminated or intrinsically complicated. However, in order to interpret the spectroscopy results, these must be compared with the appropriate theoretical calculations, such as local multiplet calculations or dynamical mean-field theory calculations, which are already highly complex challenges by themselves. In order to circumvent this problem, Tjeng and his team (MPI-CPfS, Dresden) developed a HAXPES-based technique that would allow direct imaging of the orbitals making up the band structure in crystalline solids, and thus, information about the electronic structure of correlated compounds to be obtained directly without requiring calculations [8]. Using the conventional angle-integrated HAXPES in the theoretically proposed experimental geometry (the so-called horizontal geometry in 12XU), the valence band (VB) spectra of single crystals of the model system ReO_3 were measured at many different crystallographic orientations, together with the shallow Re 4f core level. After a straightforward normalization procedure using the Re 4f core level, very strong anisotropic effects were seen in the features of the Re 5d-dominated VB [Fig. 3(a)]. From the integration of each of these features, they were able to reproduce the t_{2g} and e_g shapes [Figs. 3(b) and 3(c)] as expected from the splitting in a transition metal with octahedral symmetry.

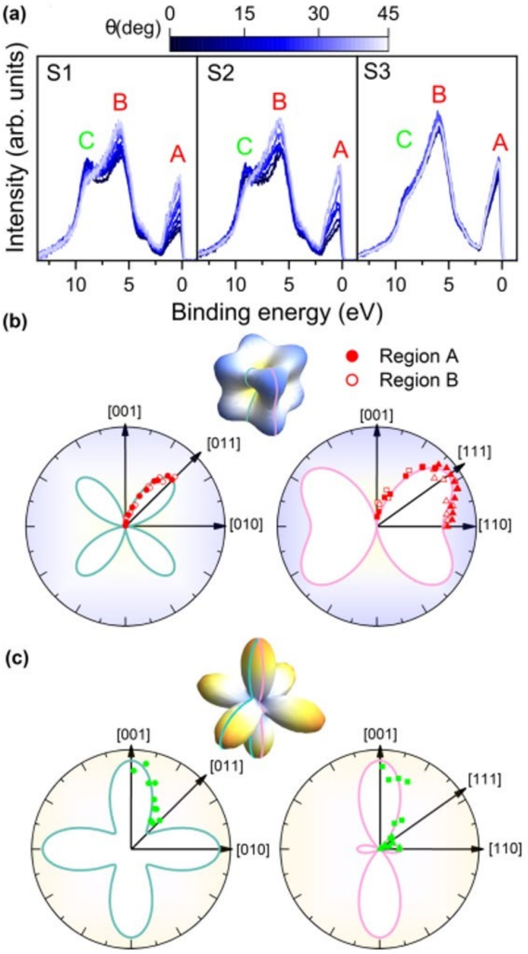

Fig. 3. (a) Valence band spectra of ReO_3 measured at various crystallographic orientations. (b)

t_{2g} shape recovered from the integral of features A and B of the valence band spectra. (c) e_g shape recovered from the integral of feature C of the valence band spectra.

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