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 another six years. The two beamlines are expected to aid research in the highenergy region, where the Taiwan Photon Source is less effective.

2. Instrumentation

The beamline major upgrading of 12XU and B2 is being performed from FY2023 to FY2026. We are expected to complete the preparations for the SPring-8-II project, that is, ring upgrading to produce brilliant synchrotron radiation. In general, the upgrading of 12B will be carried out first, followed by that of 12XU. The reason is that the optics layout of 12XU largely depends on the parameters of the synchrotron radiation ring and the insertion device that serves as the light source. We will wait for a longer period until the parameters are finalized. In FY2023, we purchased two multipixel detectors, 4M- and 0.5M-pixel CdTe sensors (Fig. 2). The pixel size is 75 μ m ×75 μ m. The former is primarily used for X-ray diffraction (XRD) experiments in B2 and partly used for coherent diffraction imaging (CDI) in 12XU. The latter will primarily be used as a detector for IXS experiments in 12XU and partly used for the dispersive X-ray absorption/emission spectroscopy (XAS/XES) experiments in 12B. We also purchased a 13element silicon drift detector (SDD) as well as 9-SDD, which will be used for XAS in 12B and may



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.

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be partly used for scanning IXS/XES experiments at 12XU.



Fig. 2. Acceptance test of the Eiger2X 500K detector. The data collection in a 4.5 ms flame time was examined with a ²⁴¹Am radioactive source.

3. Experiments

In FY2023, 31 IXS/XES and 13 HAXPES experiments were performed by general users. In total, 19 papers were published from 12XU. They include six papers on high-energy-resolution fluorescence detection (HERFD-) XAS studies of 3d/4f strongly correlated electron systems ^[1-6], five on HERFD-XAS studies of catalysts ^[7-12], three on X-ray Raman scattering, ^[13-15] three on HAXPES

studies of strongly correlated electrons, ^[16–18] and one on a HAXPES study of semiconducting functional materials ^[19]. Representative papers are briefly introduced below.

Activating dynamic atomic-configuration for single-site electrocatalyst in electrochemical

CO₂ reduction: One challenge in realizing highefficiency electrocatalysts for CO₂ electroreduction is the lack of a comprehensive understanding of potential-driven chemical state and dynamic atomic-configuration evolutions. By using a complementary combination of in situ/operando methods and employing a copper single-atom electrocatalyst as a model system, Hsu et al. provided evidence on how the complex interplay among the dynamic atomic configuration, chemical state change, and surface coulombic charging determines the resulting product profiles ^[10]. They further demonstrated an informative indicator of atomic surface charge (ϕ_e) for evaluating the CO₂RR performance and confirmed the applicability of potential-driven dynamic lowcoordination Cu centers for achieving significantly higher selectivity and activity toward CO products than the well-known four N-coordinated counterparts. This indicates that the structural reconstruction involving only the dynamic breaking of Cu-N bonds is partially reversible, whereas Cu-Cu bond formation is clearly irreversible. For all single-atom electrocatalysts (Cu, Fe, and Co), the φ_e value for efficient CO production has been revealed to be closely correlated with the configuration transformation to generate the dynamic lowcoordination configuration. The result of a universal explication indicated that the dynamic lowcoordinated configuration is the active form that

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efficiently catalyzes CO₂-to-CO conversion.

Screening response of valence and core electrons in a metal: Hiraoka et al. investigated the screening response of valence and core electrons against a test charge embedded in a metal ^[14]. The real space-andtime dynamical response function $\chi(r, t)$ was derived from the X-ray inelastic scattering spectra measured over a wide momentum and energy space on elementary Li (see Fig. 3). Embedding a charge initially induces local screening due to core electrons. This is followed by screening due to valence electrons, which exhibits an oscillatory behavior where the frequency is determined by the plasmon energy. Finally, static screening charges are produced. The static screening charge consists of a local electron cloud surrounding the embedded charge of over several angstroms, and the oscillatory charge densities have a periodicity twice that of the Fermi wave number in a larger r scale (i.e., the Friedel oscillation). The core electrons also exhibit an oscillatory behavior, where the frequency is determined by the absorption edge energy. This eventually leads to more local screening, further reducing the screening distance.



Fig. 3. Response function χ(r,t) of the screening charges, and screening charges δn (q,t) and δn (r,t) in lithium metals. δn (q,t) and δn (r,t) indicate the screening charges obtained in q-t space and r-t space, respectively.

Electronic structure of the Fe^{2+} *compound* $FeWO_4$ *:* Transition metal tungstates attract the attention of the research community owing to their remarkable electrochemical and catalytic properties. A large variety of potential technological applications such as photocatalysts, photoanodes in water-splitting reactions, electrodes in batteries, supercapacitors, electrochromic devices, and gas sensors are often discussed. In this work, Altendolf et al. focused on the iron tungstate (FeWO₄₎^[18]. The semiconducting antiferromagnet has a band gap of about 2 eV. The photoionization cross-section dependence of the elemental subshells was used to determine the different contributions to the valence band of the Fe²⁺ compound FeWO₄. From the difference between the XPS and HAXPES measurements, they extracted the position and shape of the states of the

iron and tungsten in the valence band region. A comparison of the experimental results with calculations revealed that the contribution of the iron can be well described by the full atomic multiplet configuration-interaction-based calculation for an octahedral FeO₆ cluster. A calculation of the contribution of the tungsten in a band structure model, however, shows large discrepancies. Although having an empty 5d shell, the tungsten states are not well described by a bandlike picture. This result indicates that the contribution of the tungsten cannot be derived independently by a band structure approach for the FeWO₄ because of an appreciable hybridization of W5d with Fe 3d mediated by O 2p. One rather must consider a significantly more complex model with a larger cluster that includes iron as well as tungsten octahedra in the configuration-interaction-based calculation to map the relevant correlation effects.

HIRAOKA Nozomu*, YOSHIMURA Masato, ISHII Hirofumi, and SHAO Yu-Cheng National Synchrotron Radiation Research Center (NSRRC), Taiwan

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