BL12XU
NSRRC ID

1. Overview

The contract beamline BL12XU of the National Synchrotron Radiation Research Center (NSRRC, Taiwan) has an undulator source and two branches of the mainline and a sideline. A schematic beamline layout is presented in Figure 1. The mainline has been fully operational since 2001 and used by scientists all over the world such as Japan, Taiwan, Germany, USA and so on. In 2009, like previous years, inelastic x-ray scattering (IXS) experiments were mainly performed in BL12XU but several other experiments such as high-resolution diffraction or coherent diffractive imaging were also carried out. The side line is designed to dedicate to hard-x-ray photoemission spectroscopy (HAXPES).

2. Mainline

2-1 *Instrumentation*

The resonant and nonresonant IXS spectrometers in the mainline are stably operational. Electronic excitations are studied on various kinds of samples using 5 - 10 keV x-rays. In 2010, several improvements and a performance test were made.

・**Strip detector:** we had a performance test of a new strip detector having 15 elements, each has 32 strips of 125 μm width, aiming to substantially enhance the energy resolution of the nonresonant x-ray spectrometer (Fig. 2). The resolution was successfully improved as was expected but the counting rate was much lower than a standard detector (point detector). The reasons were carefully investigated and attributed primarily to not enough bias applied.

・**Diamond phase retarder:** A thinner diamond crystal, of 300-μm thick, was newly installed for the phase retarder so that a higher transmission for x-rays was obtained in the energy range of 6 – 8 keV. Several experiments of magnetic circular dichroism were performed on iron compounds using the circular polarized beam obtained with this diamond.

・**20 keV IXS spectrometer:** Many improvements were made on the 20-keV new IXS spectrometer. A larger crystal was newly tested for a bent Laue analyzer and a reasonable performance

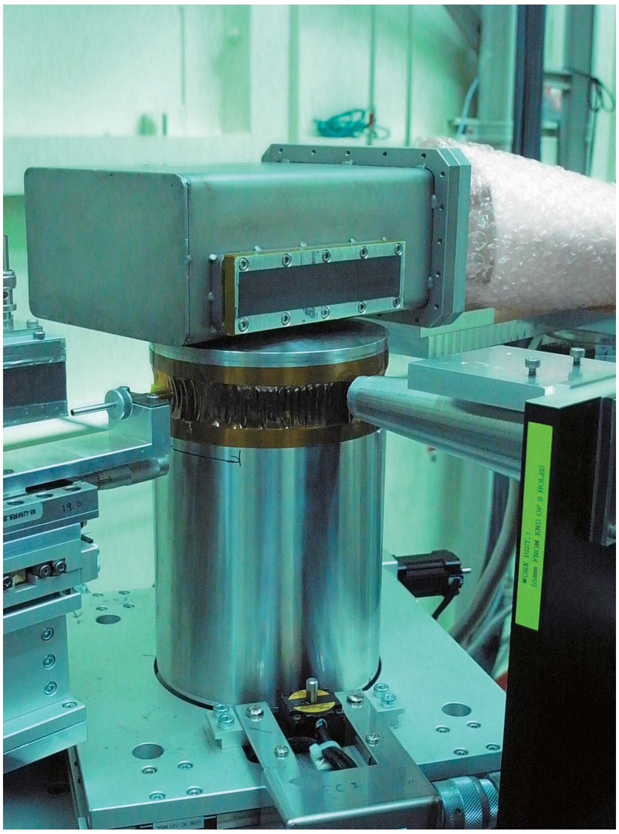

Fig. 2 Photo of a new strip detector (125 microns wide x 32 ch x 15 elements) developed for nonresonant inelastic x-ray scattering.

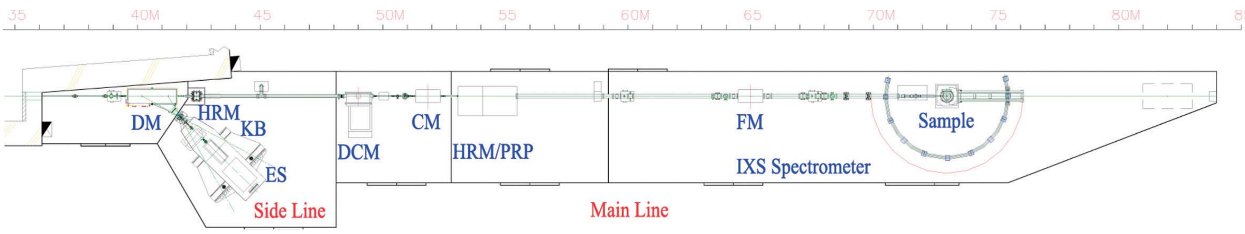

Fig. 1 Schematic layout (top view) of the BL12XU: DCM a double crystal monochromator for the main line, CM a collimating mirror, HRM a high resolution (channel cut) monochromator, PRP a phase retarding plate, FM a focusing mirror, and IXS an inelastic X-ray scattering spectrometer. For the side line DM is a diamond monochromator, HRM a high resolution (channel cut) monochromator, KB a Kirkpatrick-Baez X-ray focusing (mirrors) system; ES stands for the HAXPES end station.

was obtained in terms of energy resolution and throughput. A new tapered slits having narrower gaps for a large-area NaI detector led to better collimation so that the background was significantly reduced.

2.2 *Experiments*

In 2010, we had 10 experiments of non-resonant IXS, 3 of resonant IXS, 6 of non-resonant x-ray emission spectroscopy, 9 of resonant x-ray emission spectroscopy, 4 of coherent diffractive imaging, and 3 of high-resolution diffraction. 13 experiments were carried out under high pressure. Interesting examples are introduced below.

・**Spin crossover in (Mg,Fe)SiO_3 under high pressure:** (Mg,Fe)SiO_3 is a prototypical compound of the earth's mantle. A melt has greater volume than a silicate solid of the same composition. But this difference diminishes at high pressure and the melt can become denser because of enrichment of the heavier element iron. Nomura et al. have measured the iron partitioning by electron micro-spectroscopy and found a precipitous change at pressures greater than 76 GPa, resulting in strong iron enrichment in melts. They have also performed x-ray emission spectroscopy at BL12XU on $(Mg_{0.95}Fe_{0.05})SiO_3$ glass and indicated a spin collapse around 70 GPa (see Fig. 3), suggesting that the observed change in iron partitioning could be explained by a spin-crossover of iron in silicate melt. These results imply that (Mg,Fe)SiO_3 liquid becomes more dense than coexisting solid at 1,800 km depth in the lower mantle. Soon after Earth's formation, the heat dissipated by accretion and internal differentiation could have produced a dense melt layer up to 1,000 km in thickness underneath the solid mantle.

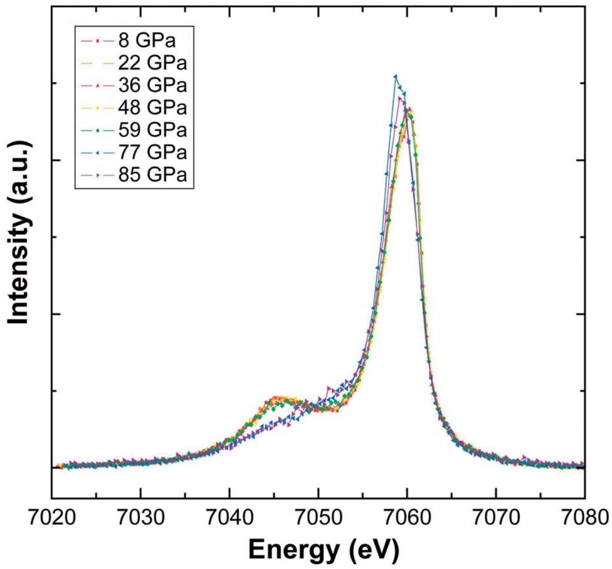

Fig. 3 Fe Kβ x-ray emission spectra from $(Mg_{0.95}Fe_{0.05})SiO_3$ (published in Nature **473** (2011) 119).

・**Magnetic circular dichroism study of resonant x-ray emission on $Sr_3Co_2Fe_{24}O_{41}$:** The magnetic circular dichroism of hard x-ray absorption at transition metal K-edge is often carried out but the subsequent x-ray emission across the absorption edge has not been fully explored yet. W.-B. Frank et al. successfully measured a large signal of magnetic circular dichroism of Fe Kβ emission at the pre-edge of Fe K-edge which has an equivalent final state of soft x-ray absorption at Fe L-edge. Further investigations are required to fully understand features in the spectra but this method is a promising tool to investigate the electronic structures of 3d magnetic samples under extreme conditions such as high pressure due to large penetration of hard x-rays compared to soft x-rays.

3. Sideline

The major development of last year was to set up the end station in two configurations with the electron emission direction either parallel to the horizontal polarization vector of incident hard x-rays or perpendicular to it, and termed horizontal or vertical geometries. The idea is to observe that the photoionization cross section of an s-orbital of 3d transition metal is very high compared to that of d-orbitals in the horizontal geometry while the s-orbital cross section tends to be suppressed in the vertical geometry. Thus the horizontal geometry can be utilized to probe chemical bonding which contains great contribution from the s-orbital while the vertical geometry used to emphasize the d-orbitals which is the origin of strong electron correlation. Figure 4 shows an example of photoemission spectra of the prototypical strongly correlated system NiO. The top spectrum is XPS using an Al Kα source. The first two peaks below the Fermi energy are typical of

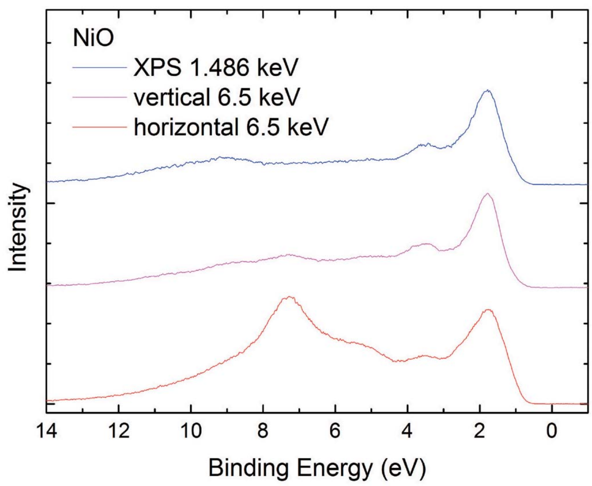

Fig. 4 Photoemission spectra of NiO using photon energy of Mg Kα (XPS) (top), 6.5 keV with a vertical geometry (center) and horizontal geometry (bottom).

photoemission spectra of NiO. However, only one peak appears in a spectrum of diluted NiO embedded in MgO (not shown). This aroused some speculation of assigning the second peak to surface effect. The central and the bottom spectra were taken at 6.5 keV photon energy with a probing depth much larger than in XPS and the two peak structure is still prominent, demonstrating it is NOT due to surface effect. Comparing spectra of horizontal and vertical geometries indicates that both peaks are primarily of d-character while s-orbital contributes more to spectral weight at higher binding energies.

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