

BL12XU NSRRC

BL12XU is one of the two contact beamlines operated by National Synchrotron Radiation Research Center (NSRRC, Taiwan). BL12XU has an undulator light source and two branches of the mainline and a sideline (see Fig.1). The mainline has been fully operational since 2001 and used by many domestic / international scientists. Inelastic x-ray scattering (IXS) experiments are mainly performed in BL12XU, and also several other experiments such as high resolution x-ray optics experiment and micro-imaging are carried out. In the side line, hard x-ray photoemission spectroscopy (HAXPES) is intensively performed. The sideline is mostly opened for users. Some adjustments and commissioning are still made by Max-Planck Institute, Dresden.

Instrumentation:

We made the following upgrading in 2017.

• KB Mirror up-grading for IXS spectrometer:

We have up-graded a KB mirror locating just before the sample position in the IXS spectrometer. The modifications are (i) a longer surface of the vertical mirror, ensuring a beam reflected in an area having a uniform curvature, (ii) a new geometry, in which a well-defined virtual source is available for the vertical focusing, (iii) a lower glancing angle, extending the x-ray energy range up to ~ 25 keV, and (iv) a replacement of dc motors with stepping motors, having a higher reproducibility of the positions and the angles. The commissioning was successfully done.

The smallest focus that we have achieved is $6 \mu\text{m}$ along the vertical axis while $28 \mu\text{m}$ in the horizontal axis. Nonetheless the vacuum pump is making a fairly large vibration, affecting the vertical focus. At present, the routinely available vertical focus is $15 \mu\text{m}$ but a further effort will be made to minimize such a vibration, so that a smaller focus will be available.

Experiments:

In 2017, we had 9 experiments of non-resonant IXS, 11 of resonant IXS (or resonant emission), 1 of high-resolution x-ray optics, 2 of micro-imaging, and 7 of HAXPES. Interesting examples are introduced below.

- Electronic structures and spin states of BaFe_2As_2 and SrFe_2As_2 probed by x-ray emission spectroscopy at Fe and As K-absorption edges:

Yamaoka et al. investigated the electronic structures of carrier-doped (electron or hole) BaFe_2As_2 and non-doped SrFe_2As_2 by resonant and nonresonant x-ray emission spectroscopy at Fe and As K-edges. They found that the electron or hole doping caused a slight enhancement of Fe K β' satellite features correlating to the local magnetic moment. Furthermore, the pre-edge peak intensity at Fe K-edge XAS spectra increased with pressure in both compounds, indicating an increase of the Fe 3d-As 4p hybridization. It was also found that pressure induced a discontinuous increase of the pre-peak intensity at As K-edge in the BaFe_2As_2 systems. These results may suggest that the Fe 3d-As 4p hybridization plays

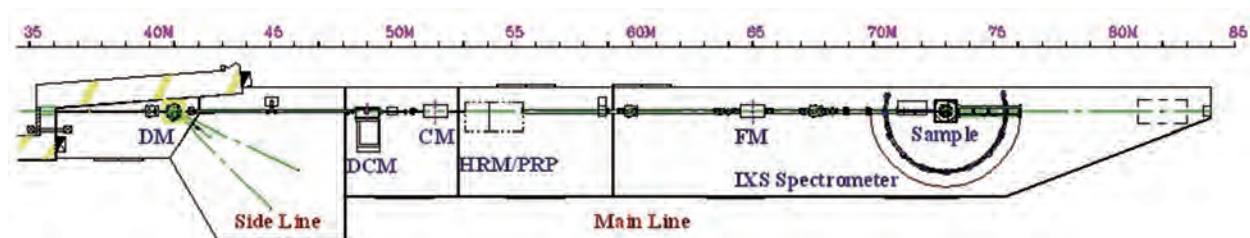


Fig.1. Schematic diagram (top view) of the BL12XU: DM is a diamond monochromator for the sideline, DCM a double crystal monochromator for the mainline, CM a collimating mirror, HRM a high resolution (channel cut) monochromator, PRP a phase retarding plate, FM a focusing mirror, and IXS an inelastic x-ray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

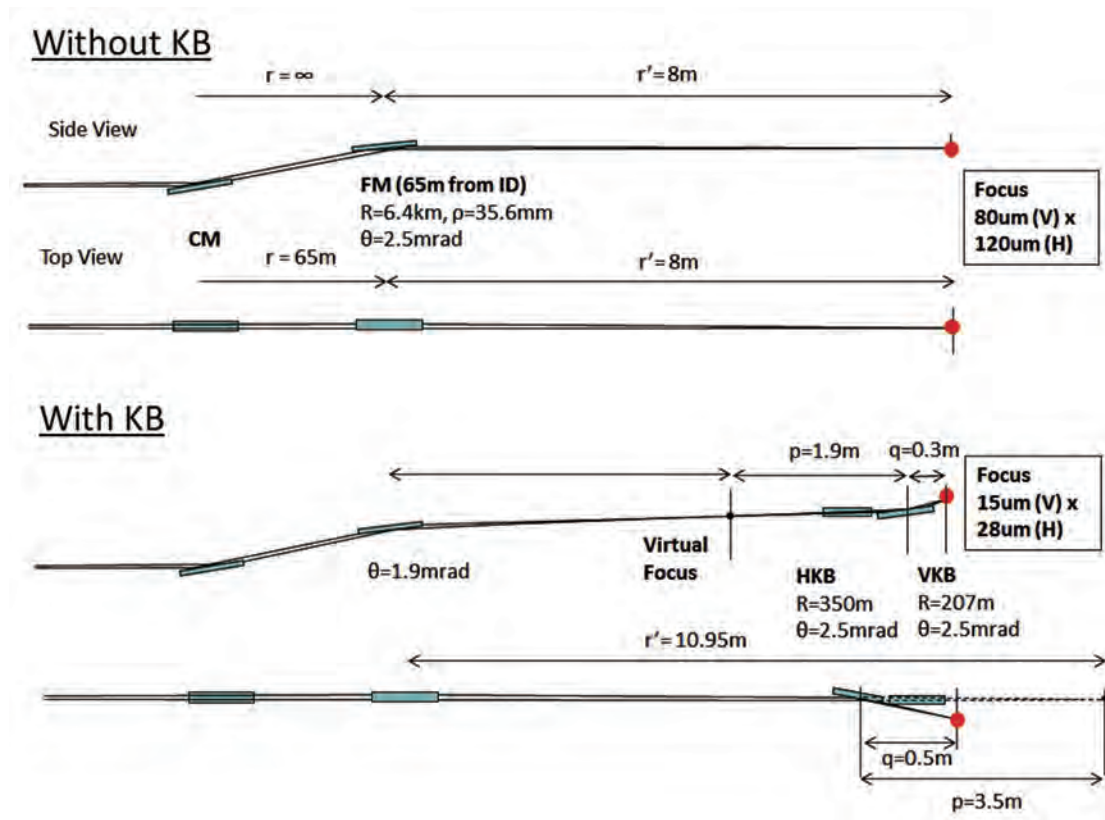


Fig.2. New geometry for the upgraded KB mirrors: Without the KB mirrors, the beam is focused into a spot of 80 μm (V) and 120 μm (H) by a cylindrical collimating mirror (CM) and a toroidal focusing mirror (FM). In the with-KB mirror mode, FM is detuned so that the beam is reflected at a smaller angle. The vertical and horizontal KB mirrors (VKB/HKB) collect the beam with a demagnification factor of about 6. Currently available beam size is 15 μm (v) x 28 μm (H).

a key role in suppressing the antiferromagnetic order by the doping or pressure and fluctuation of the local magnetic moment and the electron-electron correlation may also play a role on the physical properties of the iron superconductors. [Yamaoka et al, *Phys. Rev. B* 96 085129 (2017)]

- Electron momentum densities near Dirac cones: Anisotropic Umklapp scattering and momentum broadening:

Hiraoka & Nomura investigated the electron momentum distribution in graphite by ultra-high resolution Compton scattering (0.02-0.03 atomic units). The electron momentum distribution was significantly broadened near Brillouin zone boundaries but a sharp feature was still observable around Dirac cones. The broadening well corresponded to the magnitudes of band gaps along the zone boundaries. In fact, this effect represents a general variation of the electron densities in momentum space across the metal-insulator transitions. The experiments were performed by a newly developed x-ray Raman spectrometer using 25.5

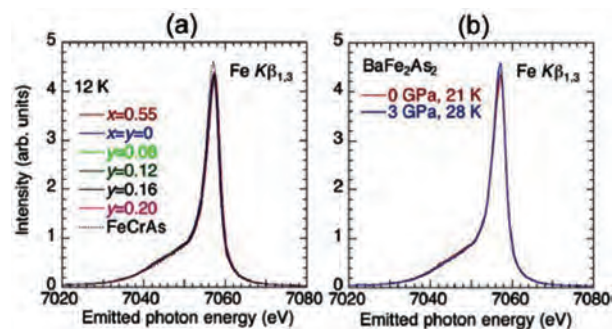


Fig.3. XES spectra of Fe compounds related to unconventional superconductors. $K\beta'$ satellite intensity provides information of the local spins in Fe ions [Phys. Rev. B 96 085129 (2017)].

keV x-rays. [N. Hiraoka & T. Nomura, *Sci. Reports* 7: 565 (2017)]

- Electronic signature of the vacancy ordering in NbO (Nb_3O_3):

Efimenko et al. investigated the electronic structure of the vacancy-ordered 4d-transition-metal monoxide NbO (Nb_3O_3) using angle-integrated soft- and hard-x-ray photoelectron spectroscopies as well as ultraviolet angle-resolved photoelectron spectroscopy.

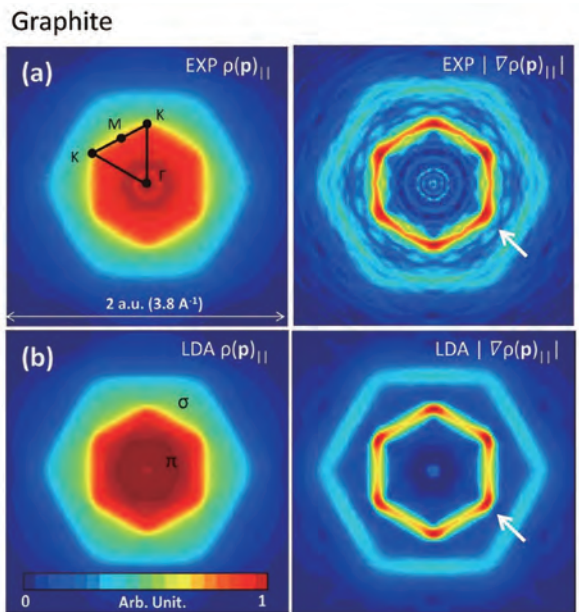


Fig.4. (Projected) electron momentum densities in graphite obtained by Compton scattering and LDA band theory. Momentum densities smoothly decay at M, where a large band gap exists, while they sharply drop at K, where the gap is closed (as in Dirac point in graphene) [*Sci. reports*, 7: 565 (2017)].

They found that the density-functional-based band-structure calculations can describe the spectral features accurately provided that self-interaction effects are taken into account. In the angle-resolved spectra they were able to identify the so-called ‘vacancy’ band that characterizes the ordering of the vacancies. This together with the band-structure results indicate the important role of the very large inter-Nb-4d hybridization for the formation of the ordered vacancies and the high thermal stability of the ordered structure of niobium monoxide. [A.K.Efimenko et al, *Phys. Rev. B* **96**, 195112 (2017)]

National Synchrotron Radiation Research Center
N. Hiraoka*, Y.F. Liao, H. Ishii, M. Yoshimura, K.D. Tsuei