

## 4-2 専用ビームライン

### BL12XU APCST ID

Following the successful completion of the initial construction and commissioning phase of the beamline and the IXS spectrometer, and in line with the scientific program envisioned for the inelastic x-ray scattering (IXS) project, the activities at BL12XU last year have been focused on improving the performance of the beamline and developing the experimental capabilities of the IXS spectrometer for performing both *non-resonant* and *resonant* IXS experiments on a variety of electronic excitations in correlated electron systems with a variable energy resolution from 10-1000 meV. A number of experiments have subsequently been performed on systems of current interest by both in-house staff and external users. We highlight some of these activities in the present report.

#### 1. Non-Resonant Inelastic X-ray Scattering (NRIXS)

NRIXS is the first major experimental capability implemented on the beamline. The incident beam energy is scanned near the close-to-backscattering energy 9.886 keV of a Si (555) analyzer crystal. The beamline configuration includes a pair of Si (333) channel-cut crystals as the high-resolution monochromator (HRM) delivering a beam of just 50 meV width at 9.886 keV. Beam intensity variation  $I/I$  after the HRM is less than 5% despite the narrow angular width of the Si (333) reflection, thanks to the greatly improved stability of the high heat-load double-crystal monochromator (DCM) through the use of a MOSTAB module that dynamically maintains the parallelism of the two crystals of the DCM. The flux of the delivered beam at the sample reaches  $1.5 \times 10^{11}$  photons/sec at 100 mA within a focus of  $75(\text{V}) \times 120(\text{H}) \mu\text{m}^2$ . Together with a highly efficient, diamond-saw diced 2-m radius Si (555) crystal analyzer, we obtain a total energy resolution of 65 meV (Fig.1). This makes the present NRIXS setup one of the most powerful in the world.

Our successful measurement of the dynamical structure of electrons in single crystal  $\text{MgB}_2$  provides a direct demonstration of this unique NRIXS capability of BL12XU.  $\text{MgB}_2$  is a simple binary compound and a superconductor with an unusually high critical

temperature ( $T_c \sim 40 \text{ K}$ ). A large number of studies have been reported since its discovery<sup>[1]</sup>, and a consistent picture has emerged of a phonon-mediated, multi-gap superconductor with strong electron-phonon coupling that conforms to conventional theory. A recent first-principle calculation of the dynamical density response function of  $\text{MgB}_2$  in particular predicted a sharp collective charge excitation in  $\text{MgB}_2$  at  $\sim 2.5 \text{ eV}$  for  $q$  along the  $c$ -axis.<sup>[2]</sup> This excitation is caused by coherent charge fluctuations between the Mg and B layers, and is believed to reflect the unique electronic structure of  $\text{MgB}_2$  that is also responsible for the strong electron-phonon coupling.

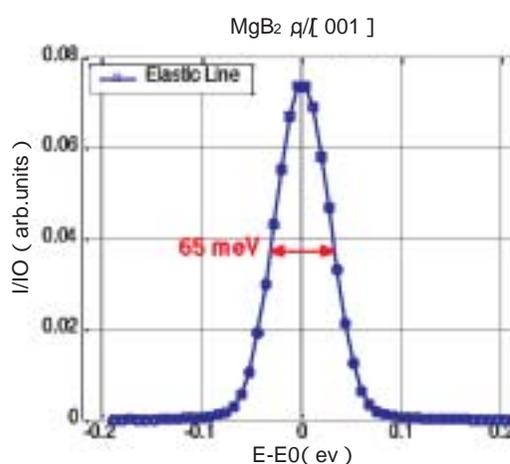


Fig.1 Quasi-elastic line obtained in the  $\text{MgB}_2$  experiment, giving a FWHM of 65 meV for the total energy resolution

Experimental effort in confirming the predicted new collective mode has been hampered by the lack of large single crystals. This problem was circumvented using the small focused and intense beam at BL12XU. The high energy resolution and sufficiently wide energy scanning range of the NRIXS setup have also played a decisive role in obtaining the experimental data shown in Fig.2, which confirm the existence of this new collective mode. The data are now under analysis and will be compared quantitatively with further calculations. Preliminary results point to an understanding of new physics in the electronic excitations of  $\text{MgB}_2$ .<sup>[3]</sup>

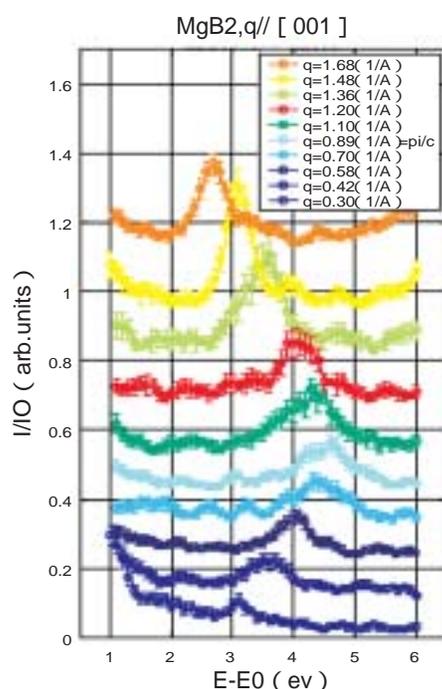


Fig.2 A collection of energy loss spectra showing the dispersion of the sharp collective mode over a range of q values with a momentum resolution of  $0.06 \text{ \AA}^{-1}$ .

## 2 . Resonant Inelastic X-ray Scattering (RIXS)

RIXS is the second major experimental capability implemented on the beamline. The DCM direct beam of used together with a 1-m radius spherically bent Ge (444) or Si (444) analyzer crystal, providing coverage of the absorption edges of Co, Ni, Cu and a few rare-earth elements. The RIXS energy can be scanned over 7.64 - 8.77 keV using the Ge (444) or 7.96 - 9.13 keV using the Si (444) by scanning the Bragg angle of the analyzer crystal and the position of the detector simultaneously while maintaining the Rowland circle geometry. The total energy resolution is about 1 eV with an incident flux of up to  $1 \times 10^{13}$  photons/sec at 100 mA. The major difference of a RIXS experiment from NRIXS is that the incident photon energy is tuned to the absorption edge of the core electrons, which leads to a large enhancement of the inelastic scattering cross

sections as demonstrated in NiO.<sup>[4]</sup> The RIXS data obtained from BL12XU on NiO are shown in Fig.3, which essentially confirm the earlier report, and demonstrate the readiness of the RIXS setup. The availability of resonant experiments at BL12XU opens up the possibility of studying secondary processes involving intermediate states as well as complex materials containing high-Z elements where sample absorption still poses a severe problem.

## 3 . Other Developments

In both types of experiments, the spherical crystal analyzer is an indispensable part of the IXS spectrometer. Several crystal analyzers with 1 or 2-m bending radii have been developed and tested,<sup>[5,6]</sup> expanding the capabilities in operating the beamline and the IXS spectrometer with different energy resolutions (see Table 1) The optimal energy resolution has to be balanced between the desire to resolve finer features with better energy resolution but less incident flux, and a higher counting efficiency with wider bandwidth and more incident flux. The appropriate energy resolution depends on the specific experiment. For studies on single-particle and collective excitations (valence and conduction electrons, plasmons and excitons, etc.) in metals, semiconductors and insulators, the optimal energy resolution would be in the range 10 - 100 meV. For near edge scattering from light elements, and measurements of the dynamical structure factor in intermediate q-regime of metals, one needs energy resolutions from about 100 meV up to 1 eV. In cases where one does not require good momentum resolution but higher energy resolution is desirable (e.g., x-ray emission spectroscopy and near edge scattering from light elements) the multiple analyzer system to be installed on the beamline will be useful. This system will be crucial also to being able to perform *non-resonant* IXS experiments of electronic excitations in high-Z materials.

Table 1 Beamline and IXS spectrometer configurations and performance of the NRIXS setup. The flux for different HRM configurations is estimated relative to the Si (333) case. The energy resolution of different analyzers is total energy resolution measured using the 50-meV incident beam from the Si (333) HRM.

Beamline			IXS Spectrometer		
HRM Configuration	Flux ( $1.5 \times 10^{11}$ photons/sec)	Bandwidth (meV)	Si(555) Analyzer	Relative Efficiency (/meV)	Resolution (meV)
Si(333)	1	50	2-m Diamond-saw Diced	25%	65
Si(440)	1.5	80	2-m DRIE Diced	-	165
Si(400)	3.8	200	2-m Continuously Bent	-	230
Si(220)	9	480	1-m Continuously Bent	-	680

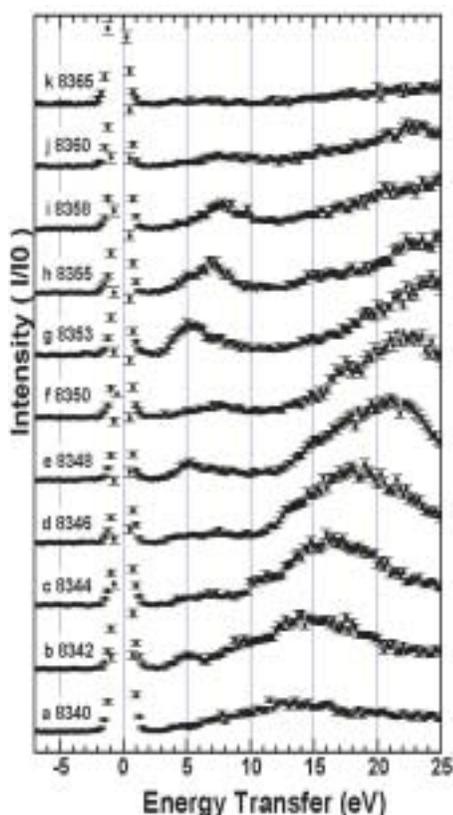


Fig.3 RIXS experimental data obtained from a NiO single crystal. The alphabets indicate the incident photon energies used to acquire the RIXS spectra, where the charge transfer excitations between 5 - 8 eV can be seen between incident photon energies of 8342 - 8360 eV.

#### Acknowledgement

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