Optical Design and Performance of the Taiwan Inelastic X-Ray Scattering Beamline (BL12XU) at SPring-8

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As part of the Taiwan x-ray facility at SPring-8, we have designed, constructed and commissioned a dedicated Inelastic X-ray Scattering (IXS) beamline for both resonant and non-resonant experiments on electronic excitations to explore frontier research in correlated electron systems with energy resolution from 10-1000 meV. The beamline optics has been designed to take full advantage of the high brilliance of the SPring-8 undulator source. At the Si(555) near-backscattering energy of 9.886 keV, a total energy resolution of 70 meV has been achieved with flux of 1.5×10^{11} phs/sec/50meV. The optical design and performance of the beamline are presented and illustrated with selected results from recent commissioning experiments.

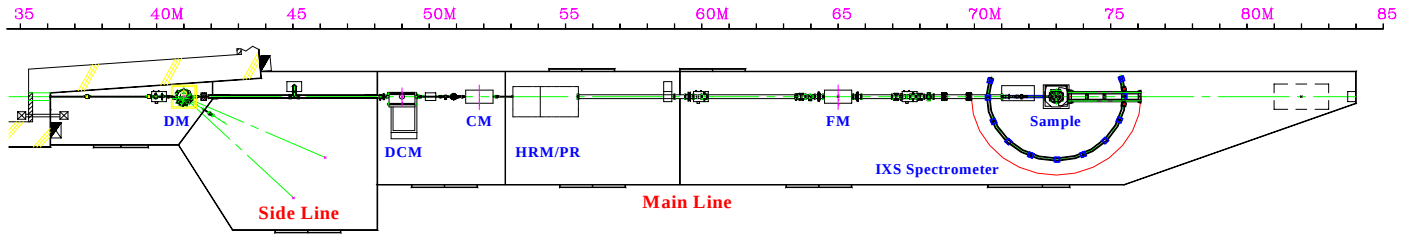
SCIENTIFIC PROGRAM

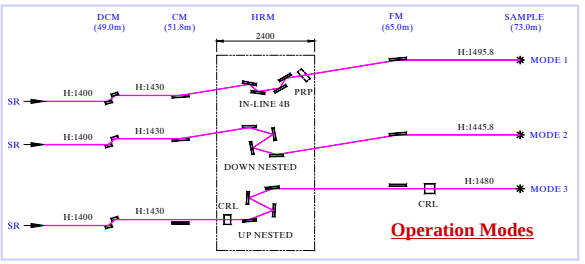
High-resolution non-resonant inelastic x-ray scattering (NRIXS)
Focus on study of various single-particle and collective electronic excitations in a variety of materials

High-resolution resonant x-ray Raman Scattering (RIXS)
Explore the large resonant enhancement of the inelastic scattering cross sections to study high-Z materials

Ultra-high-resolution inelastic x-ray scattering
Focus on the study of lattice dynamics in biomaterials and low-energy electronic excitations in strongly correlated systems

RADIATION SOURCE AND BEAMLINE DESIGN





In-Vacuum Undulator
- SPring-8 standard design 4.5 m long
- Magnet period 32 mm
- Peak field 0.85 T with K = 2.45 at 8 mm gap
- Peak total power 13.1 kW
- Peak brilliance 1.2×10^{20} phs/s/mrad^2/mm^2/0.1%BW at 9 keV

Front End
- SPring-8 standard design
- Modified total power 18 kW, providing the possibility to upgrade the undulator in the future

Side Line
- Operates in parasitic mode
- Designed for diffraction experiments or emerging experimental techniques
- Single-bounce diamond monochromator (DM)
- Energy range 8-32 keV
- Energy width ~ 1-eV

Main Line
- Designed primarily for inelastic x-ray scattering
- Energy range 5-35 keV
- Energy width 10-1000 meV
- Beam size ~ 100 μm
- Compatible with a back-scattering monochromator for 1-meV operation

DCM & CM
- High heat-load DCM with LN2 cooling, SPring-8 standard design, Si(111) reflection for 5-35 keV
- Collimating mirror, Si, cylindrical with R_m = 41.2 km and two stripes (Si: 5-12 keV & Pt: 12-30 keV) for harmonic rejection
- Beam collimation 3.3 μrad

LN2 Cooling System
- Re-circulating sub-cooled LN2 (76 K)
- Optimized flow rate 5.3 l/m
- Maximum heat load 500W (ID gap 8 mm, FE slit 1.0×1.0 mm^2)

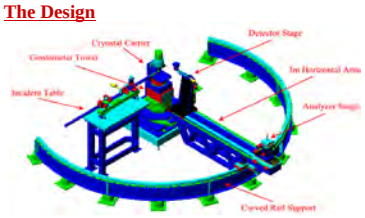
HRM/PR
- Two or four bounce (in-line or nested) channel-cut for wide tuning range with 10-100 meV resolution
- Nested four bounce for specific energies with 1-10 meV resolution
- Phase retarder (PR) to generate circularly polarized light

FM
- Focusing mirror, toroidal with R_m = 6.4 km and R_s = 35.6 mm, Si mirror with Pt coating for 5-30 keV
- Beam size at sample 120(H)×75(V) μm^2

IXS SPECTROMETER

The IXS spectrometer is basically a Rowland circle instrument with a 3-m horizontal arm. It uses spherical crystal analysers for the energy analysis of the scattered x-rays with the sample at the source and the detector at the focus of the analyser. Analysers with bending radii of 1-3 m can be accommodated. The heavy-duty goniometer tower has a load capacity for a cryo magnet. A pulse-tube cryostat with custom-built carrier provides a sample environment down to 4K.

The Design

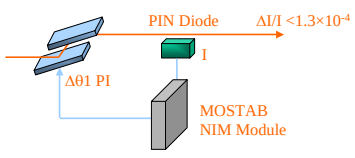


The Real Thing

Performance Indicators
- Sphere of confusion of all circles combined: ±7 μm
- Static angular stability: 10 μrad
- Analyser angular stability against arm motion: 10 μrad

PERFORMANCE

DCM Stability and Performance



Crystal parallelism is maintained dynamically using a MOSTAB module, controlling the PI piezo drive on Δθ1 based on feedback from a Si PIN diode.

Vibration Damping

- Vibration and/or heat-load induced broadening to rocking curve width: < 0.2” at 18 keV
- Total flux at sample at 9.886 keV scaled to 100 mA: 1.2×10^{13} phs/sec/1.4eV

NRIXS

Available high-resolution NRIXS setups. The energy widths of the HRM was measured using a flat Si(555) analyser. The total energy resolutions were the quasi-elastic line width of a 2-mm thick plastic sample.

Beamline			IXS Spectrometer		
HRM Configuration	Flux (×10^{11} photons/sec)	Energy Width (meV)	Si(555) Spherical Analyser	Relative Efficiency (/meV)	Total Energy Resolution (meV)
Si(333)	1.5	50	2-m diced	25%	70
Si(400)	5.7	153	2-m bent		305

RIXS

Initial setup covers the *K* absorption edges of the late transition metals (Co, Ni and Cu) using 1-m radius spherically bent analysers and DCM direct beam. The total energy resolution will later be improved to 0.2 eV with 2-m radius analysers.

Spherical Analyser	Energy Range (keV)	Total Energy Resolution (eV)
1-m bent Ge(444)	7.64-8.77	1
1-m bent Si(444)	7.96-9.13	1

SELECTED RESULTS

Dynamical Structure of Electrons in Single-Crystal MgB_2

The data on MgB_2 in Fig. 1(a) were taken at room temperature with a total energy resolution of 65 meV and a momentum resolution of 0.06 Å^{-1}. The data show clearly the dispersion of a narrow feature turning back across the zone boundary (q = 0.89 Å^{-1}) with an energy loss between 2.5-4.5 eV, which may be identified with the theoretically predicted sharp coherent charge excitation for **q** along the *c*-axis [Ku *et al*, Phys. Rev. Lett. 88, 057001 (2002)]. Comparison with further calculations may shed new light on the nature of the dynamical response of electrons in this fascinating material [Chow *et al*, unpublished].

Near K-edge Structure of Oxygen in H_2O under High Pressure and Low Temperature

The data shown in Fig. 1(b) were obtained with a total energy resolution of 305 meV at 2θ = 35°. The 2.5-kbar pressure was applied using a diamond anvil cell with Be gasket. The data reveal clearly the pre-edge features and show changes associated with the various phases. Comparison with model calculations will reveal details on the change of covalent, hydrogen, and ionic bonding of the H_2O framework that is important to understanding the icy planetary interiors as well as organic and biological materials at high pressures [Cai *et al*, unpublished].

RIXS Experiments on Transition Metal Oxides

RIXS experiments have been performed on a number of transition metal oxides with a total energy resolution of 1 eV [Ishii *et al*, unpublished]. The data obtained from NiO are shown in Fig. 2. The resonant enhancement of the charge transfer features between 5-8 eV can be seen between incident photon energies of 8340-8360 eV in Fig. 2(b). Constant final state spectra, in which the resonant behavior can be seen more clearly, are shown in Fig. 2(c). These results confirm essentially the earlier report [Kao *et al*, Phys. Rev. B 54, 16361 (1996)], and demonstrate the readiness of the RIXS setup, which 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.

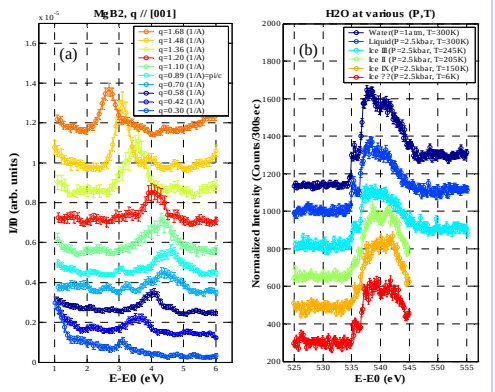


FIGURE 1. (a) NRIXS data obtained from a free-standing single crystal of MgB_2 at room temperature. (b) Near-edge scattering from the oxygen *K* edge of H_2O at various phases under high pressure and low temperature.

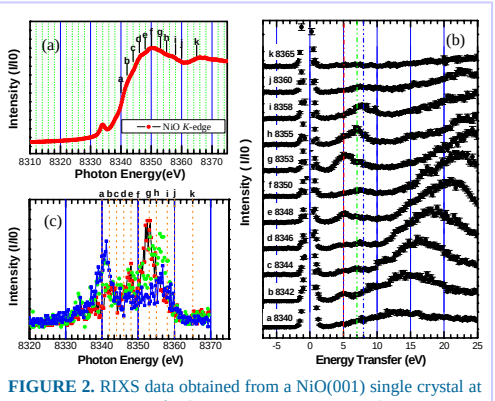


FIGURE 2. RIXS data obtained from a NiO(001) single crystal at 2θ = 30°. Constant final state spectra (c) was taken at energy transfers of 5 eV (red), 7 eV (green), and 8 eV (blue).

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