X-RAY ABSORPTION SPECTROSCOPY AND X-RAY MAGNETIC CIRCULAR DICHROISM AT PLS2-2A BEAMLINE

Jang Won
20252116

INTRODUCTION

X-ray Absorption Spectroscopy (XAS) and X-ray Magnetic Circular Dichroism (XMCD) are advanced synchrotron-based techniques widely used to investigate the electronic and magnetic properties of materials at the atomic level. These methods provide element-specific insight into unoccupied electronic states, magnetic moments, and hybridization effects in complex materials. In this experiment, conducted at the 2A beamline of the Pohang Light Source II (PLS-II), we performed XAS and XMCD measurements on NiO thin films to explore both the oxygen K-edge and the nickel L-edge. Our findings reveal detailed information about the local chemical environment and magnetic coupling between oxygen and nickel atoms.

BASIC PRINCIPLES OF XAS AND XMCD

XAS measures the absorption of X-rays as a function of photon energy. When the X-ray energy matches the binding energy of a core electron, it is absorbed and excites the electron to unoccupied states, resulting in a sharp increase in absorption known as the absorption edge. The shape and position of these edges (e.g., K-edge for 1s electrons, L-edge for 2p electrons) provide information about the oxidation state, coordination geometry, and local electronic structure.

XMCD extends XAS by utilizing circularly polarized X-rays and applying an external magnetic field. By comparing absorption spectra obtained with left- and right-circularly polarized light (or equivalently, with reversed magnetic fields), XMCD isolates the spin and orbital magnetic contributions via sum rules. The examples of magnetic moments are given by

$$m_{orb} = -\frac{4}{3}\frac{\int_{L_3+L_2}(\mu_+ - \mu_-)d\omega}{\int_{L_3+L_2}(\mu_+ + \mu_-)d\omega}(10 - n_{3d}) \tag{1}$$

$$m_{spin} = -\frac{6\int_{L_3}(\mu_+ - \mu_-)d\omega - 4\int_{L_3+L_2}(\mu_+ - \mu_-)d\omega}{\int_{L_3+L_2}(\mu_+ + \mu_-)d\omega} \times (10 - n_{3d})\left(1 + \frac{7\langle T_z\rangle}{2\langle S_z\rangle}\right)^{-1} \tag{2}$$

If necessary, the contribution of various quasiparticles such as magnons can be calculated and incorporated into the sum rule accordingly. This makes XMCD particularly powerful for studying magnetic ordering and element-specific magnetization in materials such as transition metal oxides.

EXPERIMENTAL SETUP

All measurements were carried out at the 2A beamline of PLS-II, which is equipped with an Elliptically Polarized Undulator (EPU) to generate soft X-rays with variable polarization. The beamline includes high-resolution spherical grating monochromators and focusing mirrors to control energy and beam shape. Samples were mounted in an ultra-high vacuum chamber (10 Torr) and maintained at low tem-

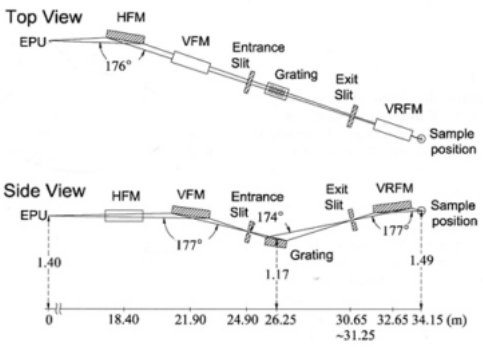

Figure 1: Schematic view of PLS-2 beamline

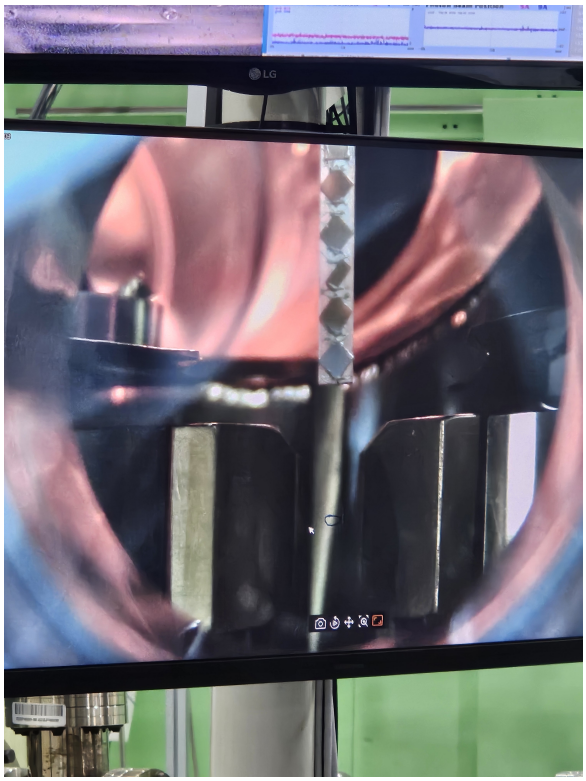

Figure 2: Sample stage of 2A-beamline: By adjusting the magnets placed on either side of the sample, the effective polarization of the incident light interacting with the sample can be controlled

peratures (5–370 K) for enhanced spectral resolution and signal stability.

For XAS, we scanned the photon energy across the O K-edge (500–560 eV) and Ni L-edge (840–885 eV), collecting data using total electron yield (TEY) and fluorescence yield (FY) detectors. For XMCD, a magnetic field was applied to the sample, and measurements were taken with fixed circular polarization while alternating the field direction to extract the dichroic signal.

RESULTS

XAS

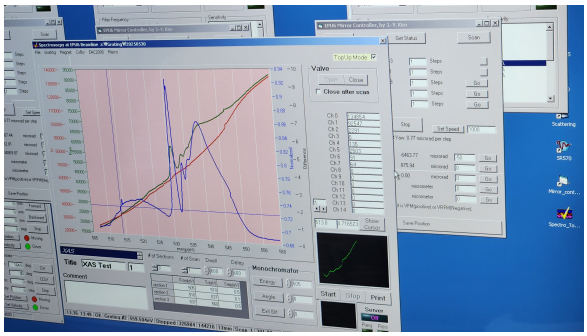

Figure 3: XAS spectrum of NiO

At the oxygen K-edge, we observed a sharp absorption peak near 530 eV, corresponding to transitions from O 1s core levels to unoccupied 2p states. The presence and shape of this peak indicate strong hybridization between oxygen 2p and nickel 3d states in the NiO lattice. This feature is sensitive to the chemical environment and oxidation state of oxygen, which confirms the structural integrity of the NiO thin films.

XMCD

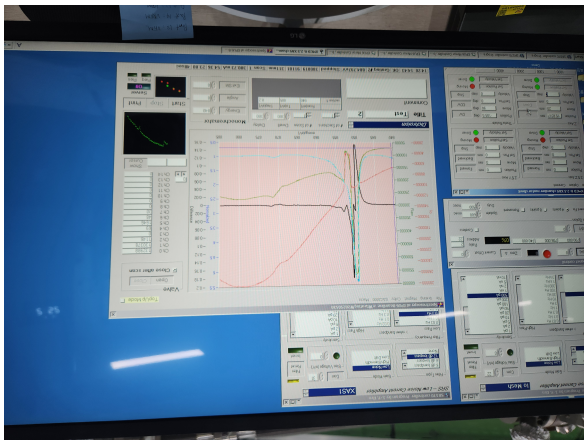

Figure 4: XMCD spectrum of NiO

XMCD spectra at the Ni L-edge revealed clear dichroic signals. A negative peak at the L edge (850 eV) and a positive peak at the L edge (853 eV) were observed, consistent with spin-polarized 2p to 3d transitions. These features demonstrate the presence of magnetic ordering in the Ni sublattice. Intriguingly, a weak XMCD signal was also detected at the oxygen K-edge, suggesting induced magnetic polarization in oxygen atoms due to hybridization with the magnetic nickel sites. This indicates interfacial magnetic coupling, which is relevant for understanding emergent properties in oxide heterostructures.

CONCLUSION

XAS and XMCD provide complementary perspectives on the electronic and magnetic structure of materials. In our study, XAS revealed the unoccupied states and chemical environment at the O K-edge and Ni L-edge, while XMCD distinguished spin and orbital magnetic contributions at the Ni site and hinted at magnetic coupling at the O site. These results not only confirm the capabilities of synchrotron-based spectroscopy but also highlight the importance of element-specific probes for understanding complex materials like NiO, which are of great interest for spintronic and quantum technologies.

REFERENCES

[1] Young-Hak Kim , *Lecture Notes on NUCE719P*, Division of Advanced Nuclear Engineering, POSTECH, PowerPoint presentation, 2025.