Probing Element-Specific Magnetism in NiO Thin Films Using Soft X-ray Spectroscopy

Dahee Jang, ID: 20252087, Div. of Advanced Nuclear Engineering, POSTECH, Pohang, Republic of Korea

Abstract

This study explores the magnetic and electronic properties of NiO thin films using soft X-ray absorption spectroscopy (XAS) and X-ray magnetic circular dichroism (XMCD) at the PLS-II 2A beamline. Measurements at the oxygen K-edge and nickel L-edge revealed insights into unoccupied electronic states and element-specific magnetism. The XMCD response at the oxygen edge indicates induced magnetism through hybridization with nickel. Experimental configurations, detection techniques, and theoretical background are presented to highlight synchrotron-based spectroscopy's capabilities in probing interfacial magnetism in transition metal oxides.

1 Introduction

Magnetic and electronic properties at the atomic level play a critical role in emerging technologies such as spintronics, energy storage, and next-generation semiconductors. Soft X-ray spectroscopic techniques—X-ray Absorption Spectroscopy (XAS) and X-ray Magnetic Circular Dichroism (XMCD)—are essential tools for element-specific characterization of such properties.

In this work, we investigate NiO thin films at the Pohang Light Source-II (PLS-II) using the 2A beamline equipped with an Elliptically Polarized Undulator (EPU). The focus lies on spectral features at the oxygen K-edge and the nickel L-edge, highlighting the electronic structure and spin-resolved magnetic behavior of the system.

2 Theory and Background

2.1 X-ray Absorption Spectroscopy (XAS)

XAS probes the absorption of photons as their energy is swept across core-level binding energies. The spectrum reveals element-specific unoccupied states and is categorized into two regimes: X-ray Absorption Near Edge Structure (XANES) and Extended X-ray Absorption Fine Structure (EXAFS). The absorption coefficient $\mu(E)$ is derived using the Beer–Lambert law:

$$I_t = I_0 e^{-\mu(E)t}, \tag{1}$$

where I_t is the transmitted intensity through a sample of thickness t.

Detection modes include total electron yield (TEY), fluorescence yield (FY), and transmission. TEY is highly surface-sensitive (depth $\sim$ few nm), whereas FY captures bulk features (depth $\sim$ hundreds of nm).

2.2 X-ray Magnetic Circular Dichroism (XMCD)

XMCD isolates magnetic contributions by analyzing the difference in absorption between left- and right-circularly polarized X-rays:

$$\mathrm{XMCD}(\omega) = \mu^+(\omega) - \mu^-(\omega). \tag{2}$$

This difference arises due to spin-polarized transitions and can be used to extract orbital and spin magnetic moments via sum rules:

$$m_{\mathrm{orb}} \propto \int_{L_3+L_2} (\mu^+ - \mu^-)\, d\omega,$$

$$m_{\mathrm{spin}} \propto \int_{L_3} (\mu^+ - \mu^-)\, d\omega - \frac{4}{3}\int_{L_2} (\mu^+ - \mu^-)\, d\omega.$$

3 Experimental Setup

Experiments were performed at the 2A beamline at PLS-II, optimized for soft X-ray studies. The EPU allows for tuning of polarization and photon energy. Monochromatized beams are focused onto the sample using spherical grating mirrors and toroidal optics.

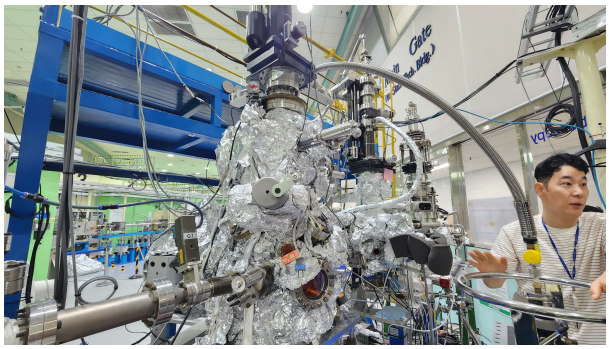

Figure 1: Schematic of the PLS-II 2A beamline and experimental end-station.

Samples were mounted in an ultra-high vacuum chamber (10^{-9} Torr). TEY was used for XAS data, while XMCD measurements were achieved by flipping the magnetic field under fixed polarization.

4 Results and Discussion

4.1 XAS at the Oxygen K-edge

XAS spectra revealed a prominent absorption peak at 530 eV, corresponding to transitions from O 1s to unoccupied 2p states. This indicates strong hybridization and provides a fingerprint for the electronic structure.

4.2 XMCD at the Nickel L-edge

XMCD spectra showed clear dichroic signals at the L_3 and L_2 edges (850–853 eV), confirming the presence of spin-polarized electronic states in Ni. A secondary XMCD feature was also observed near the oxygen edge, suggesting induced magnetism in oxygen atoms through exchange interaction.

These measurements validate the sensitivity of XMCD to element-specific magnetic ordering and underline the role of hybridization at interfaces in oxides.

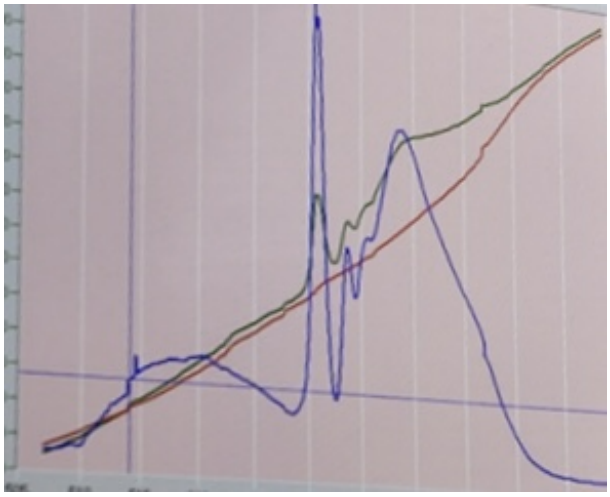

Figure 2: Oxygen K-edge XAS spectrum of NiO thin film, indicating hybridization with neighboring states.

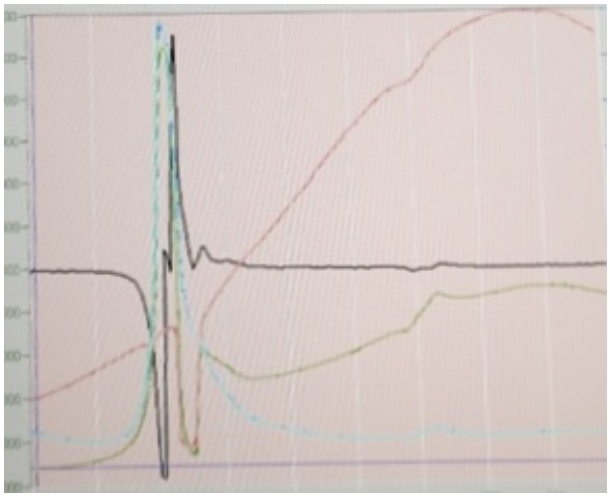

Figure 3: Nickel L-edge XMCD spectrum showing spin and orbital magnetic contributions in NiO.

5 Conclusion

The combined use of XAS and XMCD at the PLS-II 2A beamline enables detailed insights into the electronic and magnetic structures of NiO thin films. The results not only confirm the expected transition features but also highlight oxygen-induced magnetic behavior, making these methods vital for understanding magnetism in correlated oxide systems. Such insights are essential for developing spintronic and magnetoelectronic devices.

Acknowledgements

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References

[1] Y. Kim, "Soft X-ray Spectroscopy for Next-Generation Devices: Applications to AI Semiconductors and Rechargeable Batteries", Lecture Notes, NUCE719P-01, Pohang, Republic of Korea, May, 2025.