XAS AND XMCD STUDY OF ELECTRONIC AND MAGNETIC PROPERTIES IN O_2 AND NiO THIN FILMS

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Abstract

This report presents our experimental study using X-ray Absorption Spectroscopy (XAS) and X-ray Magnetic Circular Dichroism (XMCD) at the 2A beamline of Pohang Light Source II. We investigated the electronic properties of O_2 thin films with XAS and the magnetic properties of NiO thin films with XMCD. XAS measurements revealed characteristic absorption features of oxygen molecules, while XMCD measurements demonstrated magnetic properties by analyzing absorption differences between opposite magnetic field directions. The magnetic response at the oxygen absorption edge in NiO suggests induced magnetism through interaction with nickel atoms. This experiment highlights synchrotron-based spectroscopy's capabilities for investigating atomic-level material properties with applications in electronic and spintronic devices.

1. INTRODUCTION

In the previous lab, we learned how to use SAXS (Small-Angle X-ray Scattering) to study the shape and size of molecules, like proteins, in a solution [3]. SAXS helped us understand how large or compact a molecule is, but it couldn't tell us much about the material's internal properties like its magnetism or how electrons behave inside it.

In this experiment, we explored a different method called XAS and XMCD. These techniques use soft X-rays to study how materials absorb energy and how their electronic and magnetic properties behaves [2]. With XMCD, we can check how the spin and orbit of electrons contribute to a material's magnetism. These methods are useful for studying materials used in semiconductors, magnetic memory devices, and batteries [2].

During the lab, we used 2A beamline of PLS-II to send X-rays to our sample in a vacuum chamber. We learned how to prepare samples, control the undulator, and measure the signals that come out. This experiment helped us understand how X-rays interacts with matter and how we can use this to learn more about the inside of materials—not just what they look like, but also how they behave electronically and magnetically.

2. BASIC THEORY OF XAS AND XMCD

2-1. X-ray Absorption Spectroscopy (XAS)

XAS is like taking a special X-ray "photograph" of a material to see its electronic structure. When X-rays pass through a material, some are absorbed depending on the material's composition and structure. By measuring how much X-ray light is absorbed at different energies, we can learn about the material's properties.

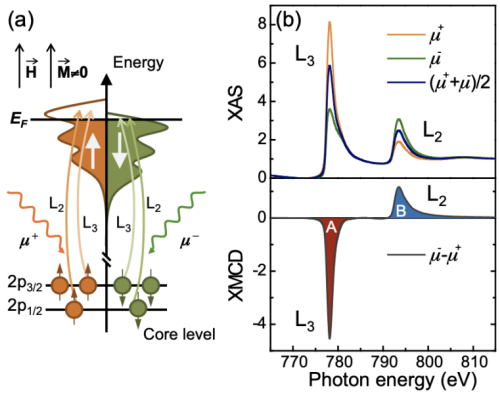

Figure 1: (a) Simplified illustration of XMCD process showing how circularly polarized X-rays interact differently with magnetic materials depending on their spin orientation. (b) Example of XAS and XMCD spectra for cobalt, showing how different X-ray polarizations (μ+ and μ-) produce different absorption patterns, and how their difference reveals magnetic properties [1].

As shown in Fig. 1(b), an XAS spectrum (the sum curve) shows how much X-ray energy is absorbed at different energy levels. The peaks in the spectrum, called absorption edges, occur when the X-ray energy matches exactly what's needed to excite electrons in the material. The position and shape of curve peaks tell us about the material's chemical state and structure.

XAS is particularly useful because it can examine specific elements within a material. For example, if we want to study just the cobalt atoms in a complex material, we can tune our X-rays to the specific energies where cobalt absorbs strongly, ignoring other elements.

2-2. X-ray Magnetic Circular Dichroism (XMCD)

XMCD builds on XAS to specifically study magnetic properties. The key difference is that XMCD uses circularly polarized X-rays either clockwise (right-handed) or counterclockwise (left-handed).

In magnetic materials, electrons have a property called "spin" that makes them act like tiny magnets. As shown in Fig. 1(a), when circularly polarized X-rays hit these spinning electrons, they interact differently depending on whether the X-ray spiral matches or opposes the electron's spin direction.

By measuring the difference between absorption of right-handed (μ+) and left-handed (μ-) X-rays, as shown in Fig. 1(b), we get the XMCD signal (the difference spectrum). This difference directly reveals information about

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the material's magnetic properties. The opposite peaks in the XMCD signal tell us about the direction and strength of magnetism in the material.

What makes XMCD special is that it can measure magnetism of specific elements within complex materials. For example, in a material containing both Ni and iron, we can separately measure the magnetic properties of just the Ni atoms or just the iron atoms by tuning the X-ray energy appropriately.

3. EXPERIMENTAL METHODS

All experiments were carried out at the 2A Elliptically Polarized Undulator (EPU) beamline of PLS-II, which is optimized for soft X-ray spectroscopy, particularly XAS and XMCD. Fig. 2 illustrates the key components of the experimental setup.

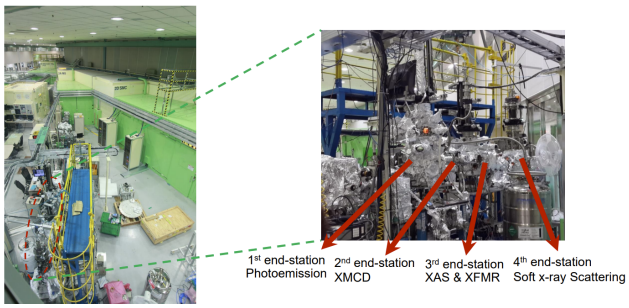

Figure 2: Schematic diagram of the experimental setup at the 2A EPU beamline [2].

Our experimental procedure consisted of three main steps: sample preparation, sample alignment, and spectroscopic measurements. As shown in Fig. 3, we first prepared thin-film samples of Oxygen (O) on silicon substrates. These samples were then mounted onto specialized sample holders and transferred into the vacuum chamber without breaking the vacuum seal. Once inside the measurement area (Fig. 3, right), we aligned both the sample position and the beam path to ensure optimal measurement conditions.

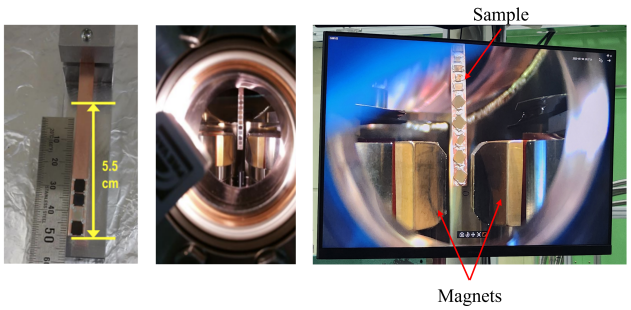

Figure 3: Sample preparation and mounting for XAS and XMCD measurements. (Left) Sample attachment process for preparing thin-film samples [2]. (Center) Inserting the fabricated sample into the vacuum chamber [2]. (Right) Sample holder positioned inside the measurement area, monitored by a camera.

For the XAS measurements, we adjusted the undulator strength and gap according to a pre-defined table of optimized values for each energy range. This allowed us to sweep the beam energy across the absorption edges of our target elements. The absorption signal was recorded as the sample drain current, which is proportional to the number of electrons ejected from the sample surface.

For the XMCD measurements, we followed a similar procedure but with an additional step of applying a magnetic field to the sample. Since XMCD requires measuring the difference in absorption between opposite magnetic polarizations (see Fig. 1), we kept the X-ray polarization fixed while reversing the direction of the applied magnetic field. This approach allowed us to collect the magnetic-dependent absorption spectra needed to calculate the XMCD signal.

4. RESULTS

4-1. XAS Measurements

Fig. 4 shows the XAS spectra we obtained from our oxygen sample. The spectrum displays characteristic absorption peaks that correspond to the excitation of electrons from core levels to unoccupied states in the material. These features provide information about the electronic structure of oxygen in our sample.

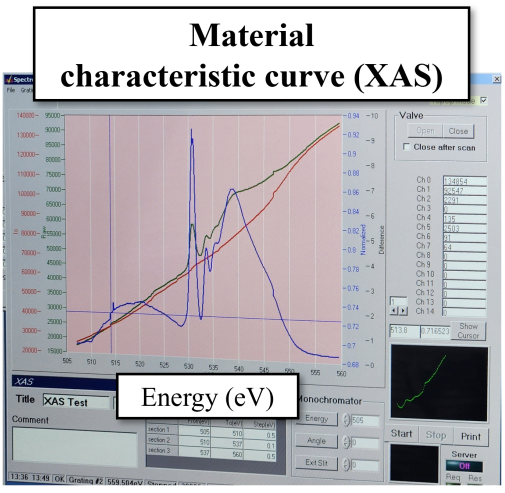

Figure 4: XAS measurement results showing the absorption spectra of oxygen. The characteristic peaks correspond to electronic transitions from core levels to unoccupied states, revealing information about the electronic structure of the sample.

In the XAS spectrum, we can observe two main regions of interest. The first peak at lower energy (around 530 eV) corresponds to transitions to the unoccupied k states of oxygen (Oxygen K-edge), while the broader features at higher energies represent transitions to higher-energy unoccupied states. The shape and intensity of these features tell us about the chemical environment of oxygen atoms in our sample.

By comparing our measured spectrum with reference data, we could confirm that our sample contained oxygen in the expected chemical state.

4-2. XMCD Measurements

After completing the XAS measurements, we proceeded to collect XMCD data by applying opposite magnetic fields to the sample while keeping the X-ray polarization fixed. Fig. 5 presents the resulting XMCD spectrum, which shows the difference in absorption between the two magnetic field directions.

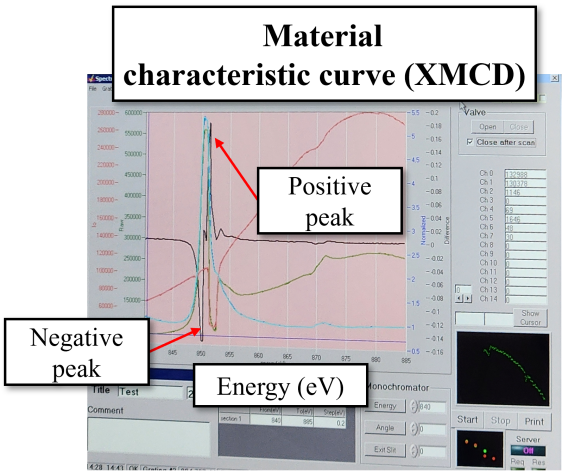

Figure 5: XMCD measurement results showing the difference in X-ray absorption between opposite magnetic field directions. The positive and negative peaks indicate the magnetic response of the sample, providing information about its magnetic properties.

The XMCD spectrum reveals magnetic dichroism with alternating positive and negative peaks. These features directly correspond to the magnetic properties of our sample. The strength of the XMCD signal (the difference between positive and negative peaks) indicates the magnitude of the magnetic moment, while the shape of the spectrum provides information about the type of magnetism present.

What's particularly interesting in our results is the clear magnetic response observed at the NiO L-edge. This suggests that NiO atoms in our sample have acquired magnetic properties, likely through interaction with neighboring magnetic elements.

By analyzing the areas under the positive and negative peaks in the XMCD spectrum, we could estimate the relative contributions of spin and orbital moments to the total magnetic moment. This analysis helps us understand the fundamental origin of magnetism in our sample at the atomic level.

5. SUMMARY

In this experiment, we conducted XAS and XMCD measurements at the 2A EPU beamline of PLS-II. Through these techniques, we were able to probe both the electronic and magnetic properties of our oxygen-containing samples. The XAS measurements revealed absorption features that provided insights into the electronic structure of oxygen atoms, while the XMCD results demonstrated the presence of magnetic properties in NiO sample. This experiment highlighted the application of synchrotron-based spectroscopy techniques for investigating material properties at the atomic level, with potential applications in the development of advanced electronic and spintronic devices. Overall, this laboratory experience provided us with valuable hands-on training in X-ray spectroscopy methods and deepened our understanding of the relationship between electronic structure and magnetic properties in materials.

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