THA APPLICATION OF THE SOFT X-RAY SPECTROSCOPY FOR NEXT-GENERATION DEVICES *

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Abstract

X-ray Absorption Spectroscopy (XAS) and X-ray Magnetic Circular Dichroism (XMCD) are powerful techniques for probing the electronic and magnetic structures of materials at the element-specific level. In this experiment, we explored the 2A Magnetic Spectroscopy beamline at PLS-II, which is optimized for soft X-ray studies using an elliptically polarized undulator (EPU) to control photon energy and polarization. Measurements were performed on oxygen and nickel compounds using soft X-rays in the energy range of 20–3000 eV. By aligning the beam and sample under ultra-high vacuum, we obtained absorption spectra in XAS and dichroic spectra in XMCD by alternating the magnetic field direction. The sample holder enabled rotation and precise positioning under magnetic field exposure, allowing spin and orbital magnetic moments to be resolved. Through these hands-on experiments, we learned how magnetic spectroscopy is implemented in beamline environments. This study highlights the importance of XAS and XMCD as key tools in understanding the microscopic origin of magnetism in cutting-edge materials.

INTRODUCTION

A synchrotron light source enables the investigation of material structures and fine fabrication processes using high-intensity light emitted as the electron bunch curve direction within the synchrotron. The synchrotron facility typically consists of a linear accelerator equipped with an electron gun, a storage ring that serves as the primary source of radiation, and multiple beamlines where various experiments are performed. From the storage ring, numerous beamlines extend outward to experimental hutches, each tailored to specific scientific applications. In this lab, we wish to focus on the X-ray Absorption Spectroscopy (XAS) and X-ray Magnetic Circular Dichroism (XMCD) in the 2A Magnetic Spectroscopy beamline at the Pohang Light Source II (PLS-II). Both of these techniques adopt a soft X-ray spectroscopy with an energy range of 20 - 3000 eV, and it interacts strongly with materials and has weak transmission. It is helpful in determining the electrical and magnetic structure of the matter.

In order to learn the experiment process in this beamline, we measured the Oxygen (O) and Nickel (Ni) compounds, investigating the spectroscopic profile. We learned how to set up the sample cosidering the optimal condition of the beam exposure and the equipment to control the sample position for sample analysis. In addition, we studied the effect of parameters such as the undulator gap which is related to the energy in the XAS measurement and the magnetic field which influences the absorption in the XMCD measurement. These hands-on experiments highlights the importance of the magnetic field in the analysis.

It is crucial to understand the principles of the beamline equipment to provide the pleasant environment to a lot of beam users who visit from various fields. For example, the magnetic properties of transition metal and rare earth compounds have been studied in this beamline, and these kinds of experiments require the elaborate magnetic control in the sample stage. Besides, many industrial electronic equipment components, such as semiconductor parts and batteries, are being researched here. Therefore, it is essential to be well-versed in the scientific mechanism of tools mentioned so far.

SOFT X-RAY SPECTROSCOPY THEORY

Vacuum ultraviolet and X-ray photons from the storage ring are among the most frequently used probes for the advanced study of the electronic and geometric structure of sample matter. The utilization of synchrotron radiation for the soft X-ray emission spectra adds several important qualities to this spectroscopy. It provides a very intense photon-excitation source, and monochromatized soft X-ray photons offer a higher degree of energy selectivity than do electrons. The soft X-ray absorption spectrum and magnetic circular dichroism by polarized light are introduced below [1].

X-ray Absorption Spectroscopy

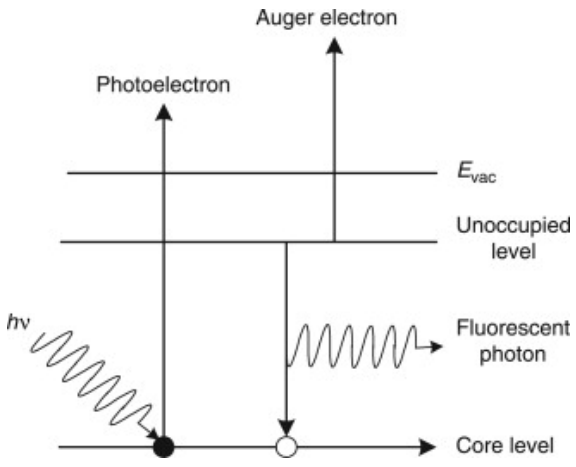

Figure 1: A diagram of energy transition as a result of X-ray absorption.

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XAS is a technique that measures how X-rays are absorbed by a material as a function of photon energy, providing information on the electronic structure, oxidation state, and local atomic environment of specific elements. It is an important tool for confirming the local geometric and electronic structure of the matter. When the X-ray beam collides with a sample, the oscillating electric field of the electromagnetic radiation interacts with the electrons in atoms of the sample. Either the radiation will be scattered by these electrons, or absorbed and excite the electrons. The intensity of the beam can be written as follows:

$$ln(I_o/I) = \mu x \quad (1)$$

where μ is the linear absorption coefficient, and it depends on the types of atoms and the density of the matter. I_0 means the initial intensity before the interaction and x is the thickness of the sample matter. The absorbed X-ray energy stimulates the electron to be excited to unoccupied level when it meets the resonance energy, $h\nu$. It can be released by either the radiation of fluorescence photons or the emission of Auger electrons. In this process, photoelectrons are measured as a function of incident photon energy [2].

X-ray Magnetic Circular Dichroism

When the XAS is extended into the field of magnetic spectroscopy, it becomes particularly powerful for investigating element-specific magnetic properties through polarization-dependent absorption. One such extension is XMCD, which measures the difference in X-ray absorption between left- and right-circularly polarized light. This difference arises due to the spin-polarized electronic structure of magnetic materials and is sensitive to the magnetic moment of specific elements. By applying a magnetic field during the measurement, XMCD enables a quantitative analysis of spin and orbital contributions to magnetism.

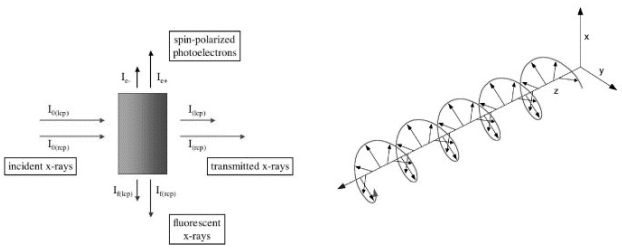


Figure 2: (Left) Schematic diagram of the XMCD experiment. (Right) Illustration of the electric field direction along the propagation axis for right circularly polarized light.

XMCD is the difference in absorption of left- and right-circularly polarized X-rays by a magnetized sample as in Fig. 2. I_0 is the incident beam intensity, I means the transmitted intensity while I_f and I_e are the intensities of the emitted fluorescence and photoelectrons, respectively. Circularly polarized X-rays have oscillating electric and magnetic fields that are 90° out of phase with each other. The polarization can be changed from left to right circular polarization in the beam with the direction of the applied magnetic field to the sample, allowing for the verification of the absorption state [3].

BEAMLINE LAYOUT

2A Magnetic Spectroscopy beamline at PLS-II is composed of four experiment stations according to each purpose: Photoemission, XMCD, XAS, and Soft X-ray Scattering. Among them, we looked around XAS and XMCD in which various matters are studied in terms of the magnetic properties.

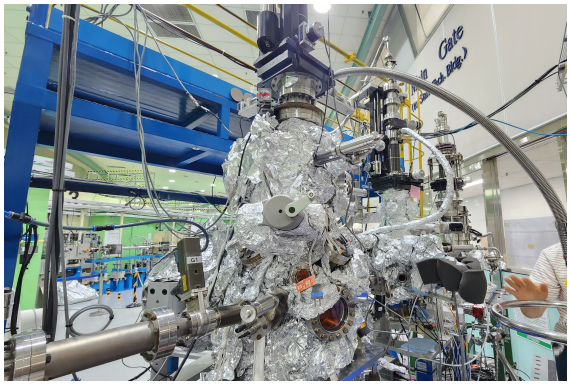


Figure 3: A whole feature of 2A beamline equipment. Sheets of Aluminium foils cover the apparatus to convey the heat in the baking process.

This beamline has an unique light source, which is an EPU (Elliptically Polarized Undulator); a special insertion device that can freely change the polarization of X-rays to linear, circular, or elliptically polarized. This makes it absolutely advantageous for studying new materials with crystal anisotropy, magnetic anisotropy, and so on, and it is also known as the EPU beamline by the reason of the characteristics of the light source. The EPU can change the photon energy by using the adjustable undulator gap in addition to the polarization state. The beam emitted from the EPU, then, passes a series of grating optics to control both the beam direction and the pathway. Finally, we can identify the beam through the fluorescer.

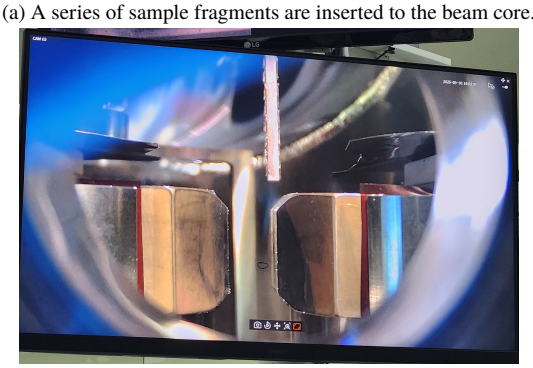
SAMPLE MEASUREMENT AND ANALYSIS

Experiment Stage Configuration

An experimental stage consists of sample installation, beam alignment, and data acquisition. When attaching samples to the holder, the electrical connection between the sample surface and the sample holder must be maintained. When controlling the beam, the alignment of the beam can be changed or regulated using the vertical focusing mirror. By adjusting the pitch of the vertical focusing mirror, the state of the photon beam passing through the entrance slit can be adjusted. Each parameter (Pitch, Roll, Yaw, X, Y) has to achieve the optimal state. Once the position of both the sample and the photon beam are aligned, measurement can

be started after the surface treatment which is suitable for each sample.

(a) A series of sample fragments are inserted to the beam core.



(b) A direction of the holder is orthogonally changed.

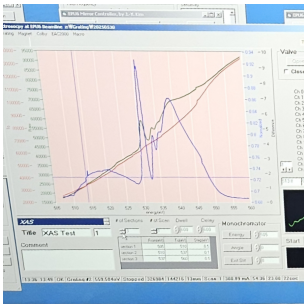
Figure 4: Sample holder adjustment apparatus.

In particular, we concentrated on the alignment of the position of the sample using a precisely controlled sample stage holder. The magnetic field is applied to the area where the sample is mounted and exposed to the beam. The holder moves down to the field so that the samples attached to the holder can be sequentially irradiated with the magnetic field and beam. Sample size is proper to be cut into 3mm x 3mm 5mm x 5mm while beam size is smaller than this, approximately 1mm x 0.2mm. A vacuum must be created inside the chamber when measuring the sample, and if the vacuum is not maintained well, the surface becomes contaminated. Baking and cooling processes take up to 18 hours to create UHV (ultra-high vacuum, 1×10^{-9} torr). Additionally, the holder can be rotated along the z-axis to alter the direction of the magnetic field, as shown in Fig. 4b.

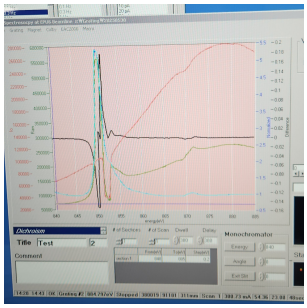
Data analysis

To investigate electronic and local geometric structures of various materials, XAS spectrum measurement is introduced. We can find out the unoccupied state of the electron as well as the ground state through the excitation of electrons. In the form of spectrums, it shows the X-ray absorption and energy transition. Briefly, it is elucidated as a finger print of the electronic states.

XMCD measurement shows the difference between circularly polarized x-rays with opposite helicities, which is induced by ferromagnetic ordering. The magnetic field where the sample is probed is reversed into the opposite direction



(a) A spectrum of Oxygen in NiO by XAS. The graph indicates the absorption and transition of the energy.



(b) Ni spectrum by XMCD. Maximum and minimum peaks are induced by the magnetic field.

Figure 5: Results of Oxygen compound spectrum measurement

while the beam polarization keeps stationary. It allows to illustrate the separation of spin and orbital magnetic moment. Furthermore, it provides the information of the geometrical magnetic properties, magnetic dichroism.

SUMMARY

Collectively, soft X-ray spectroscopy has been a key pillar supporting applied materials and basic materials science research. Rigorous and reliable spectroscopic information on basic and applied materials has provided key information for elucidating the mechanisms of switching, information storage, and batteries, and for designing future materials related to these. From these point, learning the prinicple of the spectroscopy and beamline control is of importance in delevoping much more technologies. We studied XAS and XMCD spectroscopy which present the electric and magnetic properties of the matter in a subatomic scale. XAS and XMCD have the nature of element and polarization depending on the materials; they can delve into specific energy levels and magnetism in microscopic origin. In order to proactively discover and apply various future materials in the future, it is essential to provide more abundant and sophisticated challenging spectroscopic information. To this end, we have to discuss and reestablish the utilization goals and demands for high-quality synchrotron radiation from a future perspective.

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