

## Electronic structure of dilute magnetic semiconductor $\text{Fe}_x\text{Nb}_y\text{TiO}_{2-x-y}$ studied by XAS and XMCD

Toshihiro SHIMADA<sup>1\*</sup>, Hitoshi ABE<sup>1</sup>, Takumi OHTSUKI<sup>1</sup>, Enju SAKAI<sup>1</sup>, Hiroyuki NOGAWA<sup>1</sup>, Taro HITOSUGI<sup>1</sup>, Kenta AMEMIYA<sup>2</sup>, Tetsuya HASEGAWA<sup>1</sup>

<sup>1</sup>Department of Chemistry, The University of Tokyo, Tokyo 113-0033, Japan

<sup>2</sup>Photon Factory, High Energy Accelerator Research Organization (KEK), Ibaraki 305-8001, Japan

### Introduction

Oxide dilute magnetic semiconductors (DMS) are gathering much attention since their discovery[1] and yet there are still arguments on the origin of the magnetism. We measured X-ray magnetic circular dichroism (XMCD) and X-ray absorption spectroscopy (XAS) of a group of those materials,  $(\text{Fe or Co})_x\text{Nb}_y\text{TiO}_{2-x-y}$  [2-4]. It is considered that local spin of Fe or Co is the origin of the magnetism whereas Nb provides n-type carriers that induce the ordering of the spins of magnetic dopants (Fe and Co). The position of the Ti 3d level is very important in the magnetic polaron model[5]. Nevertheless the energy levels of dopants have not been measured directly and it has been awaited in order to elucidate the origin of the magnetism.

### Experiments

The samples were prepared by pulsed laser deposition epitaxial growth technique on  $\text{SrTiO}_3(001)$  or  $\text{LaAlO}_3(001)$  substrates. X-ray diffraction of the sample showed the epitaxial growth of anatase  $\text{TiO}_2$  structure. XAS and XMCD were measured at BL-7A under high vacuum ( $\sim 3 \times 10^{-6}$  Pa) under the magnetic field of  $\pm 2000\text{G}$ . Remanent condition after the application of the magnetic field was also used for the measurement. The XAS and XMCD signals were detected by using total electron yield technique with an extraction bias electrode. It is established that the n-type carrier concentration is nearly proportional to the Nb dopant concentration[4].

### Results and Discussions

The experimental results so far suggest the relationship between energy levels in this system as shown in Fig. 1. Energy levels of  $\text{Fe}^{2+}$  and  $\text{Fe}^{3+}$  lie close to the partly filled Ti 3d band. The energy levels of Nb dopant and oxygen deficiency are also close to the Fermi edge. Figure 2 shows the Ti L- XAS and XMCD of  $\text{Fe}_{0.06}\text{Nb}_{0.03}\text{TiO}_2$ . It shows a weak indication of XMCD signal which is negative in sign. This result shows that the spin polarization in Ti is opposite to that in Fe, and is consistent with the magnetic polaron model.

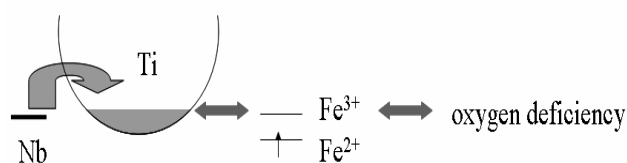


Fig.1: Relationship between energy levels of chemical species in  $\text{Fe}_x\text{Nb}_y\text{Ti}_{1-x-y}\text{O}_2$ , determined by the XMCD and XAS experiments.

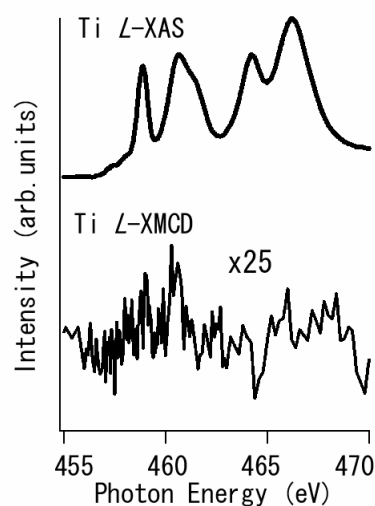


Fig.2: Ti L-XAS of  $\text{Fe}_{0.06}\text{Nb}_{0.03}\text{TiO}_2$

### References

- [1] Y. Matsumoto et al., Science 291,854 (2001).
- [2] T.Hitosugi et al., J.Appl.Phys.99,08M121(2006).
- [3] K. Inaba et al.,Jpn.J.Appl.Phys.45,L1141(2005).
- [4] G. Kinoda et al., Jpn.J.Appl.Phys.45,L387(2006).
- [5] J.M.D. Coey et al., Nature Mater.4, 173(2005)

\* shimada@chem.s.u-tokyo.ac.jp