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Local distortion in a Ni-doped TiO_2 semiconductor

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We report the x-ray diffraction, x-ray absorption fine structure and magnetization study for Ni-doped TiO_2 magnetic semiconductors. We have observed the local distortion around the impurity atom in the diluted magnetic semiconductor.

1. Introduction

Dilute magnetic semiconductor oxides with a ferromagnetic behavior above room temperature are investigated extensively for applying to spintronics devices [1]. Some models have been proposed for ferromagnetism of the oxides in which defects, especially oxygen vacancies, play an important role [2]. We have detected the oxygen vacancies in the room temperature ferromagnet Co-doped TiO_2 by XAFS measurements [3]. We here report on XAFS for a Ni-doped TiO_2.

2. Experiment

The Ni-doped TiO_2 was synthesized by the solid state reaction from the mixture of rutile-type TiO_2 (99.99%) and NiO (99.97%). They were milled and annealed at 800 ^oC for 20 h in air.

We measured XAFS of Ni-doped TiO_2 and rutile-type TiO_2 at the Photon Factory to investigate the electronic states and the local structure. X-ray diffraction and magnetic hysteresis measurements were also carried out at room temperature.

3. Results and Discussion

Any other peaks than those of the rutile-type phase (space group P42/mnm) are not observed in x-ray diffraction patterns. We determine the lattice constants from the Rietveld analysis of x-ray diffraction, which decreases with increasing the Ni content. The magnetization measurement shows that they are ferromagnetic at room temperature.

Figure 1 shows the radial structural function around Ti atoms for TiO_2. A peak around 1.5 Å corresponds to Ti-O pairs, the second one around 2.5 Å is for the Ti-Ti bond and the third peak around 3.0 Å consists of Ti-O and Ti-Ti pairs. These peaks are characteristic of the rutile-type structure.

Figure 2 represents the radial structural function around Ni atoms for 5%Ni-doped TiO_2, which shows that the doped Ni atom is substituted for the Ti site of the rutile type TiO_2 matrix. The x-ray absorption near edge structure measurement shows the valence of the substituted Ni to be 2+. The interatomic distance between Ni and O is by about 0.05 Å larger than that of the Ti-O bond in the Ni-doped TiO_2, which is as same as that of the TiO_2 matrix. That is, the O neighbor keeps away from the Ni atom. This may relate both of the Ni valence of 2+ and the charge neutrality.

In conclusion, we have observed the local distortion around the impurity atom in the diluted magnetic semiconductor, which is much different from the average lattice structure measured by x-ray diffraction.

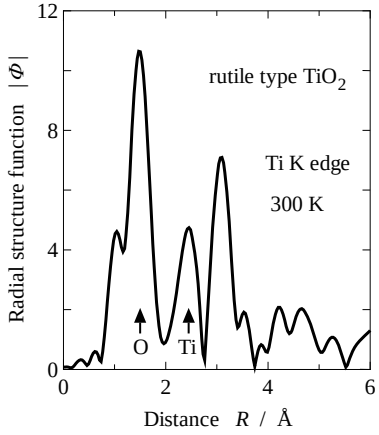

Fig. 1: The radial structure function of a rutyle-type TiO_2 for the Ti K edge at 300 K.

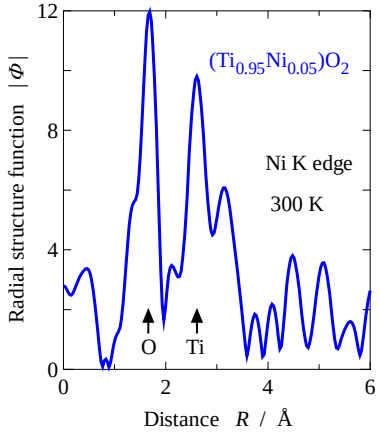

Fig. 2: The radial structure function of $(Ti_{0.95}Ni_{0.05})O_2$ for the Ni K edge at 300 K.

References

[1] Y. Matsumoto *et al*., *Science* **291**, 854 (2001).
[2] J. M. D. Coey *et al*., *Nature Mater*. **5**, 173 (2005).
[3] I. Nakai *el al*., *J. Korean Phys. Soc.* **63**, 532 (2013).

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