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Polarization-dependent Ti *K* x-ray absorption and emission studies of Ti_2O_3 single crystal

Hiroyuki MASO[1], Hidenao KURIHARA[1], Yutaka MUKAEGAWA[1], Yuki UTSUMI[1], Hitoshi SATO[2], Yasuhisa TEZUKA[3], Toshiaki IWAZUMI[4], Fumitoshi IGA[5], Masami TSUBOTA[6], Hirofumi NAMATAME[2] and Masaki TANIGUCHI[1,2]
[1]Graduate School of Science, [2]HiSOR, [5]ADSM, [6] Graduate School of Integrated Arts and Sciences, Hiroshima University, Higashi-Hiroshima [1]739-8526, [2]739-0046, [5]739-8520, [6]739-8521, Japan
[3]Graduate School of Science and Engineering, Hirosaki University, Hirosaki 036-8561, Japan
[4]Graduate School of Science, Osaka Prefecture University, Sakai 599-8531, Japan

Introduction

Ti_2O_3 exhibits a metal (high-temperature phase) - insulator (low-temperature phase) transition (MIT) around 450 K. The Ti 3*d* levels in Ti_2O_3 split into the t_{2g} and $e_g{}^{\sigma}$ levels. Due to the trigonally distorted crystal field, the t_{2g} level further splits into the $e_g{}^{\pi}$ and a_{1g} levels. Tanaka has proposed a new MIT model taking into account the many-body effect and predicted that the Ti 3*d* configuration of the Ti ion pair along *c*-axis changes from ($a_{1g}\uparrow$, $a_{1g}\downarrow$) in the insulating phase to ($a_{1g}\uparrow$, $e_g{}^{\pi}\uparrow$) in the metallic phase [1]. Recently, we have detected the 3*d* configuration change due to MIT by means of polarization-dependent Ti 2*p*-3*d* absorption spectroscopy [2]. In this report, we present the polarization-dependent Ti *K* x-ray absorption and emission (XAS and XES) spectra of Ti_2O_3 single crystal.

Experiment

The Ti *K* XAS and XES experiments were carried out at BL-7C and BL-15B1 with polarized and depolarized configurations for XES, respectively. ESCARGOT with a Ge(400) crystal and a PSPC detector were used to measure the XES spectra. Both spectra were measured with ***E***//*c* and ***E***⊥*c* conditions, where ***E*** denotes a polarization vector of incidence light. Note that the Ti ion pair is parallel to the *c*-axis. Experimental data presented here is taken at room temperature.

Results and discussion

An upper side in Fig. 1 shows Ti *K* XAS spectra of Ti_2O_3. Thick and thin curves represent spectra measured with ***E***//*c* and ***E***⊥*c* conditions. One notices that a feature of the XAS spectra is different between two conditions. Peak energy of a white line of the ***E***//*c*–spectra is lower than ***E***⊥*c*–spectra by about 2 eV and a clear shoulder is found just below the white line. This difference shows a remarkable anisotropy in the unoccupied Ti 4*p* states of Ti_2O_3. The lower energy of the $4p_{//}$ bands than the $4p_{\perp}$ bands contradicts our intuition, considering the a_{1g} states is mainly occupied.

A lower side in Fig. 1 shows the ***E***//*c*- and ***E***⊥*c*- XES spectra in the K_α region measured at 4958.3 eV, far below the Ti K-edge, with polarized configuration. Abscissa is denoted by the Raman shift. Interestingly, the polarization-dependent Raman spectra are very similar to the K XAS spectra with respect to the energy shift and the shoulder structure. This experimental result suggests that the structure of the Raman spectra originates from the 2*p*-4*p* transition. This trend is also found for TiO_2 single crystal [3].

Features of the XES spectra strongly depend on the excitation energy below 4964 eV and show several fine structures depending on the ***E***//*c* and ***E***⊥*c* conditions. Detailed analysis is in progress and experiments above 450 K is also planned.

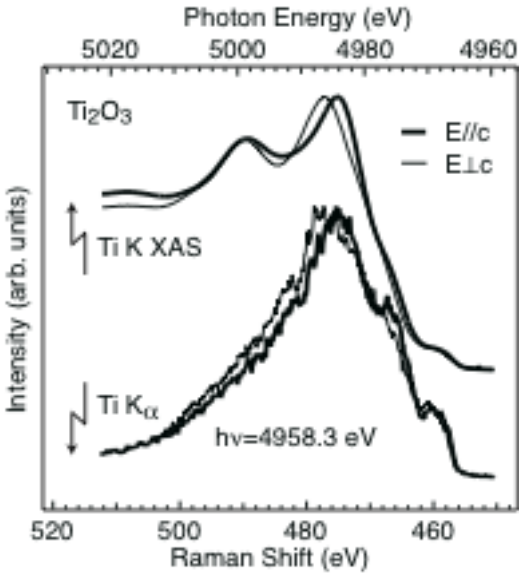

Fig.1. Polarization-dependent Ti K XAS and Raman spectra of Ti_2O_3. The Raman spectra were measured at 4958.3 eV, far below the K-edge.

References

[1] A. Tanaka, J. Phys. Soc. Jpn. 73, 152 (2004).
[2] H. Sato et al., J. Phys. Soc. Jpn. 75, L053702 (2006).
[3] Y. Tezuka, private communication.

*jinjin@hiroshima-u.ac.jp