

Studies of Electronic Structure for $\text{Ti}_{1-x}\text{V}_x\text{O}_2$

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INTRODUCTION

Titanium vanadium oxides, including $\text{Ti}_{1-x}\text{V}_x\text{O}_2$ rutile solid solution have been attracting much attention because of their application in display devices, color filters, smart windows, lithium cells and many oxidation and reduction reactions. They are used as electrodes [1], electrochromic materials [2], and catalysts [3]. In order to explain the electronic, electrochromic, and optical properties of titanium vanadium oxides, it is very important to study their electronic structure. So far, there is neither theoretical nor experimental studies for electronic structure of titanium vanadium oxides, has been reported.

X-ray spectroscopy is a powerful technique for the study of the electronic structure of solids and the characterization of materials. The soft x-ray emission spectra (SXES) are capable of yielding occupied partial density of states in valence band for solid systems, whereas the x-ray absorption spectra reflect the unoccupied partial density of states. The disadvantage of SXES spectroscopy is the typically low fluorescence yields for many core levels, particularly for light elements. However, nowadays, the synchrotron radiation sources has stimulated the interest in the study of soft x-ray emission using photon excitation [4]. Advanced Light Source can overcome many of the disadvantages of electron spectroscopies. For example, it not only offer the high brightness that makes high resolution SXE experiments practical, but also allows a detailed investigation of defined materials by changing the excitation energy.

EXPERIMENTAL RESULTS

The SXES for $\text{Ti}_{1-x}\text{V}_x\text{O}_2$ were excited by photons from undulator beamline 8.0 at the Advanced Light Source in Lawrence Berkeley Laboratory, and the x-ray absorption spectra were measured from beamline 6.3.2. The Ti $L_{2,3}$ x-ray emission spectra from $\text{Ti}_{0.8}\text{V}_{0.2}\text{O}_2$ are shown in Fig. 1. It can be seen that the spectra are almost the same as that of TiO_2 (rutile) [5]. An elastic peak, a main peak and Raman scattering peak can be found in Fig. 1. The main peak located a energy about 453 eV should be a L_3 spectrum which results from transitions from the valence band to the $2p_{3/2}$ core hole of Ti atom. The Ti $L_{2,3}$ x-ray absorption spectrum is shown in Fig. 2. For comparison, the Ti $L_{2,3}$ x-ray absorption spectrum from TiO_2 (rutile) is also projected. Comparing the Ti $L_{2,3}$ x-ray absorption spectra from TiO_2 and $\text{Ti}_{0.8}\text{V}_{0.2}\text{O}_2$, it is found that peak positions are almost the same, however, the intensity ratio of the peaks are very different. This result indicates that quantity of the unoccupied Ti 3d states is different between TiO_2 and $\text{Ti}_{0.8}\text{V}_{0.2}\text{O}_2$. More detail experiments and theoretical calculations are necessary to clarify the electronic structure of $\text{Ti}_{0.8}\text{V}_{0.2}\text{O}_2$.

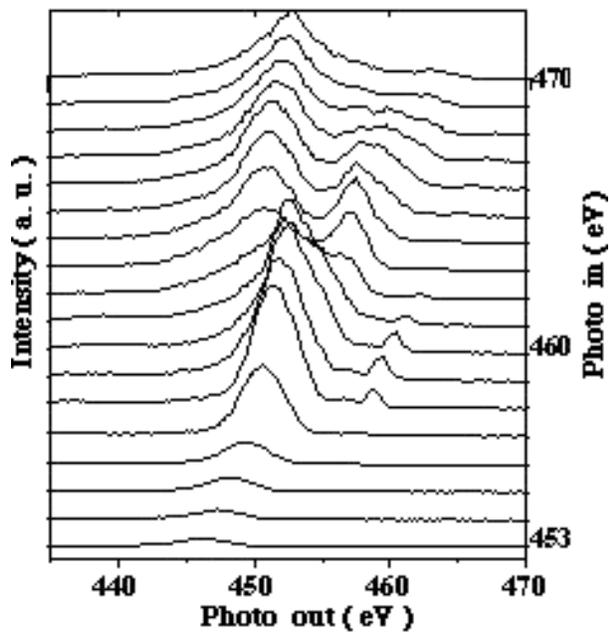


Figure 1. Evolution of the Ti $L_{2,3}$ emission spectra from $Ti_{0.8}V_{0.2}O_2$. All curves show the normalized x-ray emission as a function of the emission energy plotted as the abscissa. The scale on the right give the excitation energy.

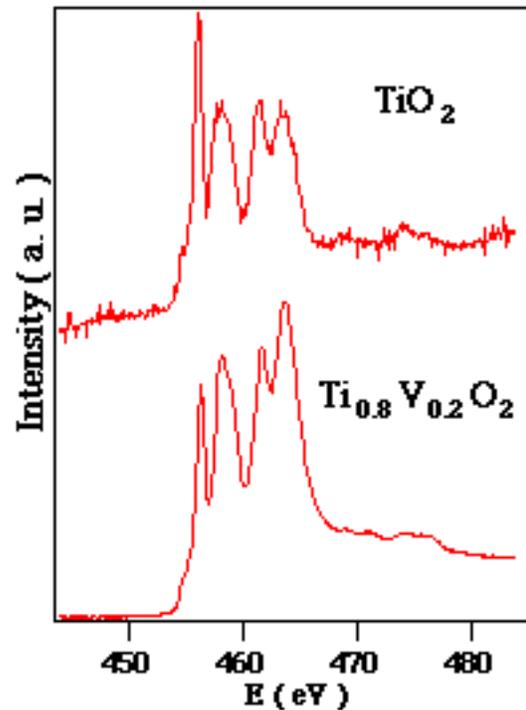


Figure 2. Comparison of the Ti $L_{2,3}$ x-ray absorption spectra between TiO_2 and $Ti_{0.8}V_{0.2}O_2$.

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This work was supported by the Division of Electronics and Applied Physics, Osaka Electro-Communication University, Japan.

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