

Soft x-ray absorption and emission study on anisotropy of electronic structure of MoO<sub>3</sub>

Yutaka MUKAEGAWA<sup>1</sup>, Hitoshi SATO\*<sup>2</sup>, Hidenao KURIHARA<sup>1</sup>, Hiroyuki MASO<sup>1</sup>,  
Yasuhisa TEZUKA<sup>3</sup>, Osamu MORIMOTO<sup>2</sup>, Hiroshi NEGISHI<sup>4</sup>, Saiko NEGISHI<sup>2</sup>,  
Hirofumi NAMATAME<sup>2</sup> and Masaki TANIGUCHI

<sup>1</sup>Graduate School of Science, <sup>2</sup>HiSOR, <sup>4</sup>ADSM, Hiroshima University,

Higashi-Hiroshima <sup>1</sup>739-8526, <sup>2</sup>739-0046, <sup>4</sup>739-8530, Japan

<sup>3</sup>Graduate School of Science and Engineering, Hirosaki 036-8561, Japan

### Introduction

Layered material MoO<sub>3</sub> is composed of an equivalent Mo atom and three inequivalent O1, O2 and O3 atoms, bonding with the Mo atom along *b*-, *c*- and *a*-axes. According to SR powder x-ray diffraction measurements, the O ionic states and Mo-O bonding nature depend on the O sites, indicating high anisotropy of its electronic structure [1]. In this study, we have deduced the anisotropy of the O 2*p* states of MoO<sub>3</sub> by means of O 1*s* soft x-ray absorption and emission spectroscopy (XAS and SXES).

### Experiments

The O 1*s* XAS and SXES experiments were carried out at BL-2C. To deduce the anisotropy of the electronic structure, XAS and SXES spectra were measured with changing polarization vector *E* of the incident light; *E*//*a*, *E*//*b* and *E*//*c*. In addition, the angular-dependence of the SXES spectra were collected with polarized and depolarized configurations (see Fig. 2).

### Results and discussion

Figure 1 shows XAS spectra of MoO<sub>3</sub> measured with *E*//*b* and *E*//*c*. We find that the feature of the spectra strongly depends on the experimental condition. In particular, the absorption edge of the *E*//*b* spectrum is about 0.5 eV lower than that of the *E*//*c* spectrum. These results indicate that the conduction-band minimum is composed mainly of the O 2*p<sub>b</sub>* states. In comparison with the band-structure calculation [2], the O 2*p<sub>b</sub>* states come from the O2 atom.

The feature of the SXES spectra depends on the excitation energy and the spectra also exhibit a

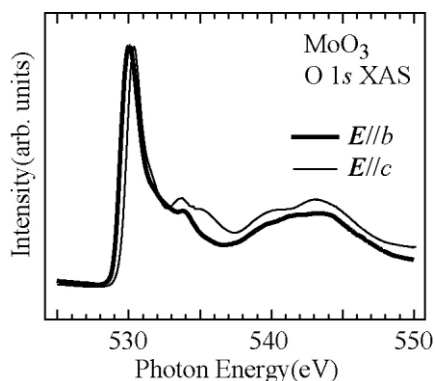


Fig. 1. XAS spectra of MoO<sub>3</sub>.

remarkable angular-dependence around the O 1*s* absorption peak, reflecting the anisotropy of the O 2*p* states. The observed angular-dependences depend on the experimental conditions; *E*//*b* and *E*//*c*, and also polarized and depolarized configurations. The dependence for all cases gradually vanishes with increasing the excitation energy and the SXES spectra become close to the fluorescence spectra, the bandwidth of which is in good agreement with the band-structure calculation [2].

As an example, Fig. 2 shows the depolarized SXES spectra for *E*//*b* measured at  $h\nu=529$  eV, 1 eV below the absorption peak for *E*//*b*. The spectra reflect the O 2*p* states in the valence bands. Emitted photon energy of  $\sim 527$  eV corresponds to the Fermi level and the binding energy becomes deep with increasing emitted photon energy. We find elastic peaks at 529 eV. The SXES spectra depend on the incidence angle  $\alpha$ . It should be noted that the 2*p<sub>a</sub>* and 2*p<sub>c</sub>* components are active for  $\alpha=70^\circ$ , while the 2*p<sub>b</sub>* and 2*p<sub>c</sub>* components for  $\alpha=20^\circ$ . The peak at 526 eV is observed only for case of  $\alpha=70^\circ$  and *E*//*b*. The same results are obtained for the polarized configuration and we conclude that the O2 2*p<sub>b</sub>* states contribute to the valence-band maximum (VBM) of MoO<sub>3</sub>. A feature of the SXES spectra above the absorption peak shows that the O3 2*p<sub>c</sub>* states also contribute to VBM and O1 2*p<sub>b</sub>* states are located around 6 eV below VBM.

### References

- [1] Y. Kuroiwa et al., J. Phys. Soc. Jpn. 72, 2811 (2003).  
[2] C. A. Rozzi et al., Phys. Rev. B68, 075106 (2003).  
\*jinjin@hiroshima-u.ac.jp

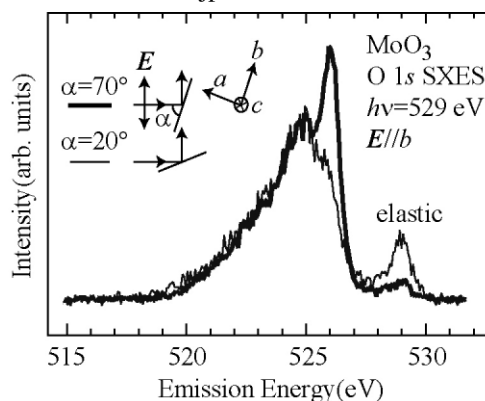


Fig. 2. Depolarized SXES spectra of MoO<sub>3</sub>.