Surface State Analysis of TiO_2(110) Sputtered with Different Element Species

Rintaro Hori, Naoyuki Maejima, and Masaru Takizawa
Department of Physical Sciences, Faculty of Science and Engineering, Ritsumeikan University, 1-1-1 Noji-Higashi, Kusatsu 525-8577, Japan

Molecular orientation of pentacene on rutile TiO_2 (110) substrates can be controlled by modifying the reduced TiO_2 [1]. In the experiment, the reduced TiO_2 was obtained by cleaning (sputtering and annealing) the rutile TiO_2 (110) surface in ultrahigh vacuum. In this study, in order to control the surface state of TiO_2 (110), sputtering using two elements was carried out and the surface electronic states were observed by near edge X-ray absorption fine structure (NEXAFS) and ultraviolet photoelectron spectroscopy (UPS).

NEXAFS and UPS measurements were performed at the BL-8 of SR Center Ritsumeikan University, equipped with a grazing incidence monochromator with a varied-line-spacing plane grating. He^+ sputtering (0.5 kV, 20 mA, 40 min) and Ar^+ sputtering (0.75 kV, 20 mA, 40 min) were performed on the cleaned substrate. NEXAFS measurement was carried out at room temperature in ultrahigh vacuum of 2×10^{-7} Pa. NEXAFS spectra were recorded in partial electron yield mode. UPS was performed at ~10^{-7} Pa.

Figure 1 shows UPS spectra of the TiO_2 surfaces. Selective sputtering removes oxygen from the surface and donates electrons to the surface. As a result, the surface electron density increases, and excess electrons are trapped in Ti 3*d* orbitals. The peak around 0.9 eV indicates that electrons are trapped in Ti 3*d* orbitals. The peak is prominent in Ar^+ sputtering, and appear slightly in He^+ sputtering.

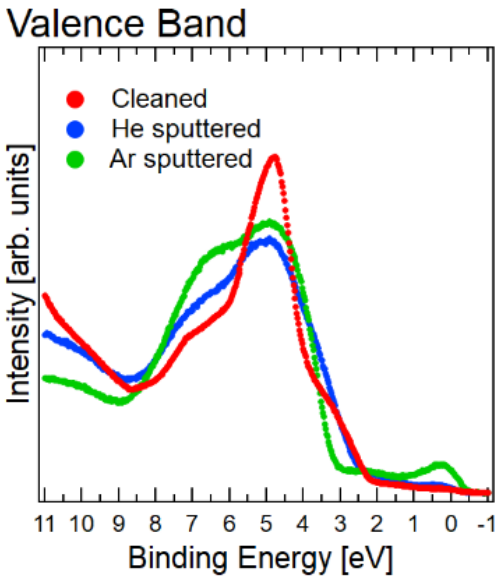

Fig. 1 UPS spectra for various surface state TiO_2.

Figure 2 shows NEXAFS spectra of the TiO_2 surfaces. Figure 2 (a) shows the Ti *L*-edge spectra. In the case of clean TiO_2, the splitting of t_{2g} and e_g orbitals is characteristic of the crystal structure [2]. After Ar^+ sputtering, the splitting disappears, indicating that appearance of Ti^{3+} component. After He^+ sputtering, the orbital splitting is maintained, which suggests that the Ti^{4+} state is preserved. Figure 2 (b) shows the O *K*-edge. The characteristics of the O *K*-edge are consistent with those of the Ti *L*-edge.

In this study, sputtering was performed using different elemental species and the effects were compared. Significant differences were observed between Ar^+ and He^+, suggesting the possibility that different surface conditions can be tuned by changing the sputtering elemental species.

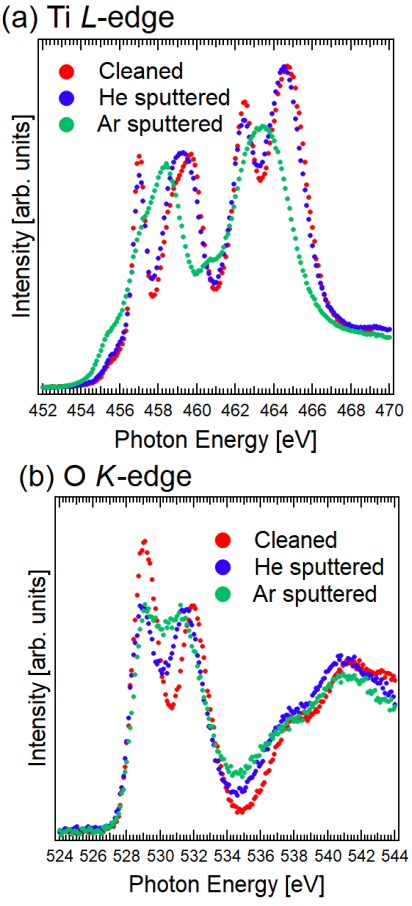

Fig. 2 XAFS spectra of TiO_2. (a) Ti *L*-edge. (b) O *K*-edge.

References

[1] T. Sugie, Master thesis (2024).
[2] S. O. Kucheyev *et al.*, Phys. Rev. B. **69**, 245102 (2004).