Atomic and Electronic Characterization of Lattice-Work Structure on Rutile TiO_2(001) via AFM, KPFM, and STM

Eiichi Inami[1, #], Seiga Koga[1], Linfeng Hou[2], Fengxuan Li[2], Daiki Katsube[3] and Masayuki Abe[2]

[1] *School of Systems Engineering, Kochi University of Technology, 185 Miyanokuchi, Tosayamada, Kami, Kochi 782-8502, Japan*
[2] *Graduate School of Engineering Science, The University of Osaka, 1-3 Machikaneyama, Toyonaka, Osaka 560-8531, Japan*
[3] *Japan Fine Ceramics Center, 2-4-1 Mutsuno, Atsuta, Nagoya 456-8587, Japan*

Presenting author's e-mail: inami.eiichi@kochi-tech.ac.jp

Titanium dioxide (TiO_2) is widely studied for photocatalysis, with particular attention to its crystal facets where surface nanostructures act as active sites. Among rutile TiO_2 surfaces, the (001) plane is the least stable due to low coordination of surface atoms, leading to thermal reconstruction. A notable reconstruction is the lattice-work structure (LWS)[1], which is relevant for visible-light-driven photocatalysis [2]. Although spectroscopic studies have offered insights into its electronic properties, their limited spatial resolution has prevented a direct correlation between atomic arrangement and electronic states, crucial for understanding its photocatalytic function. In this study, we investigated the atomic and electronic structures of the LWS on rutile TiO_2(001) using ambient atomic force microscopy (AFM), Kelvin probe force microscopy (KPFM), and ultrahigh-vacuum scanning tunneling microscopy (STM)[3].

AFM revealed that annealing the (001) surface generates short, bright rows aligned along the [110] and [1$\bar{1}$0] directions, which gradually elongate and eventually cover the surface. Tuning the annealing conditions thus allows control over the LWS coverage. Simultaneous AFM and KPFM mapping of the partially reconstructed surface (Figure 1a) showed that the rows are more negatively charged than the surrounding terraces, indicating localized charge accumulation. STM and scanning tunneling spectroscopy (Figure 1b) further revealed a site-dependent electronic structure: the topmost rows exhibited a narrower band gap (~1.75 eV), while the valley between the rows retained a wider band gap (>3.0 eV). These results directly link the atomic structure to its local electronic states, offering mechanistic insight into its photocatalytic role. Moreover, controlling LWS coverage via annealing provides a strategy to tune the band gap distribution for optimizing photocatalytic performance under specific wavelengths of light.

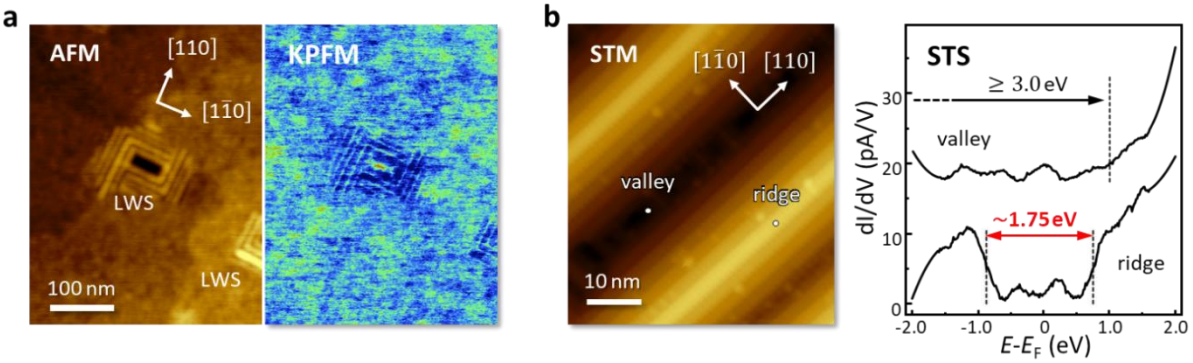

Figure 1. LWS on rutile TiO_2(001) surface characterized by AFM, KPFM, and STM.

Reference

[1] L. E. Firment, Surf. Sci. **116**, 205 (1982).
[2] H. Ariga, et al., J. Am. Chem. Soc. **131**, 14670 (2008)
[3] E. Inami, et al., Appl. Surf. Sci. Adv. **25**, 100777 (2025).