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High resolution STM imaging of a unit cell of SrTiO₃(100)- $\sqrt{5} \times \sqrt{5} - R26.6^\circ$ surface superstructures ICHIRO SHIRAKI, University of Yamanashi, KAZUSHI MIKI, National Institute for Materials Science (NIMS), SHUHENG PAN, University of Houston — SrTiO₃(100)- $\sqrt{5} \times \sqrt{5} - R26.6^\circ$ surfaces were studied by scanning tunneling microscope (STM) in ultra-high vacuum conditions at room temperatures. In our previous report, we showed the arrangement of titanium and oxygen atoms in the unit cells of a ($\sqrt{5} \times \sqrt{5}$) surface superstructure with scanning tunneling microscope and concluded the TiO₂ layer is the terminating plane of the ($\sqrt{5} \times \sqrt{5}$) surface [1]. Recently, we succeeded in imaging the surfaces in filled states with much higher spatial resolution. Oxygen atomic orbitals are individually recognized and the local structures at the center of the O fourfold hollow site with ($\sqrt{5} \times \sqrt{5}$) periodicity are more clearly seen. Comparing our experimental results with the previous works, especially a theoretical study of O-vacancy model [2] and an experimental and theoretical study of Sr adatom model [3], detailed discussion on $\sqrt{5} \times \sqrt{5}$ surfaces became possible.

[1] I. Shiraki and K. Miki, Surf. Sci. 605, 1304(2011)

[2] Z. Fang and K Terakura, Surf. Sci. 470, L75(2000)

[3] T. Kubo and H. Nozoye, Phys. Rev. Lett. 86, 1801(2001)

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