Reconsideration of SrTiO₃(100)\(-\sqrt{5}x\sqrt{5}\)-R26.6 surfaces - existence of O-vacancy and Sr adatom

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SrTiO₃(100)-\(-\sqrt{5}x\sqrt{5}\)-R26.6 surfaces were studied by scanning tunneling microscope (STM) in ultra-high vacuum conditions. The results suggest the existence of O-vacancies on the surfaces, which have not been confirmed experimentally so far. In occupied states observations of -1.2 V sample bias voltage, a pair of dangling bonds of Ti atoms neighboring an O vacancy is clearly seen as an oval shape protrusion that can be resolved apart into two protrusions, which is consistent with previous theoretical study by spin polarized LDA+U calculations [1]. Making a comparison between occupied states and unoccupied states (-1.2 V sample bias voltage) in the same scan area, the oval shape protrusions present dark contrast, which is also consistent with the theoretical study. The present proposed surface structural model requires the existence of Sr adatoms as reported by Kubo et al. [2] [1] Z. Fang and K Terakura, Surf. Sci. 470, L75(2000) [2] T. Kubo and H. Nozoye, Phys. Rev. Lett. 86, 1801(2001)