

# Structural Analysis of SrTiO<sub>3</sub> (001) Surfaces by Medium Energy Ion Scattering and Ultraviolet Photoelectron Spectroscopy

Yoshiaki Kido, Tomoaki Nishimura, Atsushi Ikeda\* and Hidetoshi. Namba

## Abstract

The structure change of TiO<sub>2</sub>-terminated SrTiO<sub>3</sub>(STO)(001) surfaces after annealing in an O<sub>2</sub> atmosphere ( $1-5 \times 10^{-6}$  Torr) and ultrahigh vacuum (UHV) was studied by ultraviolet photoelectron spectroscopy (UPS), reflection high energy electron diffraction (RHEED) and medium energy ion scattering (MEIS). The TiO<sub>2</sub>-terminated SrTiO<sub>3</sub> (001) surfaces were prepared by chemical treatment with an HF-NH<sub>4</sub>F buffer solution (pH: 3.5 - 3.8). The fraction of the TiO<sub>2</sub> face was estimated to be  $88 \pm 2$  % from the MEIS analysis. For the STO surface annealed in UHV at temperatures higher than 650°C, the surface state induced by O vacancies in the top TiO<sub>2</sub> plane was observed by UPS and the RHEED pattern shows a 2×2 structure. On the other hand, the STO surface annealed in the O<sub>2</sub> atmosphere ( $5 \times 10^{-6}$  Torr) has a 1×1 structure without O vacancies. The MEIS analysis revealed that annealing at 650°C in UHV decreased the fraction of the TiO<sub>2</sub> face by about 5 % and the O-vacancy fraction in the TiO<sub>2</sub> face was about 7 % . The present results indicate that O vacancies are initiated in the random sites of the top TiO<sub>2</sub> plane by UHV annealing and rearrangement of the atomic configuration occurs simultaneously to reduce the surface energy and thus the newly ordered 2×2 structure appears.

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*Department of Physics, Faculty of Science and Engineering, Ritsumeikan University, Kusatsu, Shiga-ken 525-8577, Japan*

*\* Present Address:*

*Matsushita Electronic Corporation, Nishikujo-Kasugacho, Minami-ku, Kyoto 601-8413, Japan*