Investigation of the SrTiO$_3$ (100) (R5xR5)R26.6° surface by means of LEED, XPD and XPS

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Strontium titanate is seeing increasing interest in fields ranging from thin-film growth to water-splitting catalysis and electronic devices. Although the surface structure and chemistry are very important to many applications, theories about the driving forces vary widely[1,2]. We prepared SrTiO$_3$(100) surface by heating produced by the passage of an electric current in UHV at high temperature of around 900°C. The as-prepared sample were characterized using XPS and LEED. The LEED experiment shows a (R5xR5)R26.6° reconstruction. We investigated the atomic structure by x-ray photoelectron diffraction (XPD) using the Sr3p$_{3/2}$ core level. In this work we have compared the results of photoelectron calculations of SrO and TiO$_2$ terminated of SrTiO$_3$(100) including relaxation and rumpling, with the experimental data. We found that for the TiO$_2$ terminated surface SrTiO$_3$(100) all top-layer cations relax inward, whereas second-layer atoms relax outward. Using a genetic algorithm the best agreement to the experimental XPD data is obtained for a TiO$_2$ terminated surface with two domains rotated by 90 degrees. The XPD simulations are in agreement with STM results[3].