

Abstract

Reconstructions on Strontium Titanate (110) Surfaces at Various Annealing Conditions

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Strontium titanate (SrTiO_3) is a perovskite complex metal oxide used in many different applications due to its tunable multifunctional properties. Understanding the surface dynamics of strontium titanate is crucial for the engineering and design of functional structures. Research on the polar SrTiO_3 (110) remains relatively scarce and findings from different groups vary greatly. Several ($n \times 1$) reconstructions in which the reconstruction type depends on sample preparation and treatment conditions were observed. In this study, reconstructions on air-annealed SrTiO_3 (110) were examined using transmission electron diffraction and microscopy. It was observed that samples annealed in air between 875°C and 1050°C for 5 hours reconstructed with a (1x5) type reconstruction. At 1150°C , the sample showed (1x4) and (1x5) reconstructions after 3 hours, but displayed a (5x1) periodicity instead after 5 hours. Annealing at 1250°C for 5 hours resulted in a fully reconstructed (5x1) periodicity. Measured electron diffraction amplitudes of the (1x5) reconstruction coupled with direct method analysis provided reasonable initial estimates of the true surface structure. Peaks refinement and density functional theory calculations narrowed down the possible solution set to several structures that seem highly possible. Currently there is a model that matches all known constraints but no conclusive results have been reached. More ongoing work is being done to solve the structure.