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Exploring surface phase, morphology, and charge distribution transitions of perovskites: a case study on SrTiO3

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The structure and properties of perovskite substrates have attracted substantial interest due to material's popularity as a substrate for complex oxide epitaxy [1,2]. Strontium titanate (SrTiO3) is among the most popular perovskites, with film quality dependent on the structure of the substrate at the beginning of the growth process. Here, we examined the surface structure of SrTiO3 (100) single crystals as a function of annealing time and temperature in either oxygen atmosphere or ultra-high vacuum (UHV) for a variety of different preparation schemes using scanning probe microscopy, auger electron spectroscopy (AES), and low-energy electron diffraction (LEED) [1]. We find that the SrTiO3 surface evolves depending on the preparation scheme with respect to surface roughness, surface terminations, and surface reconstruction. Non-contact atomic force microscopy (NC-AFM) images, e.g., reveal a non-monotonic trend of surface roughness with respect to UHV annealing temperature. Interestingly, the surface roughness changes also as a function of the bias voltage applied to the surface. This can be explained by the effect of the electrostatic field induced by both the Nb-doping and oxygen deficiencies in the bulk or on the surface, with the latter being a function of the preparation history. As for surface termination, we observe for initially TiO2-terminated crystals the formation of terraces with half unit cell step heights between them with increasing UHV annealing temperatures, implying that multiple terminations are forming. This conclusion is corroborated by AES data, which expose an increase in Sr amount relative to Ti and O. Complementary LEED data reveals a structural phase transition from (1x1) termination to an intermediate c(4x2) surface reconstruction to ultimately a sqrt(13) x sqrt(13)-R33.7° surface phase by annealing the sample with oxygen flux, while the inverse structural phase transition from sqrt(13) x sqrt(13)-R33.7° to c(4×2) is observed when annealing in UHV. As a result, we suggest that careful selection of preparation procedure combined with applying an appropriate bias voltage during growth may be used to control outcomes of thin film growth.

[1] O. E. Dagdeviren *et al.*, Physical Review B **93**, 195303 (2016).

[2] O. E. Dagdeviren *et al.*, Advanced Materials Interfaces **4**, 1601011 (2017).

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