

Revealing atomic structures and imaging modes on anatase TiO₂ (101)

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The atomic structure of the anatase titanium dioxide (101) is investigated using non-contact atomic force microscopy (NC-AFM) and charge force microscopy (CFM). Natural and synthetic anatase crystals usually accommodate impurities or dopants like Nb and images obtained by SPM measurements reveal surface and subsurface irregularities, however, their identification is challenging. Images obtained in a quasi-constant height mode reveal details of the deeper atomic rows and allow an accurate identification of O_{2c}, O_{3c}, Ti_{6c}, and Ti_{5c} positions. A series of frequency shift (Δf) NC-AFM images in figure (a-c) show a distance dependent contrast with superimposed model of the anatase atomic structure and with decreasing tip surface distance the major contribution to the contrast can change from O_{2c} rows to O_{3c} rows. Topographic (z) NC-AFM images in figure (e-g) show that the atomic structure is imaged with different contrasts as an effect of changing tip terminations which usually appear when the tip scans over surface defects. Irregularities originally imaged as bright protruding features in figure (e) change to dark hole like features in figure (f-g) and vice versa. Within these contrast changes, irregularities change from bridge position to on top position indicating that the major contrast contribution changes from oxygen to titanium rows. We identify two distinct imaging modes. In contrast I, defects are imaged as protrusions and appear as bright spots between the atomic rows. In contrast II, defects are imaged as being directly on top of the atomic rows. Topographic images in figure (f-g) further show mobility for some irregularities. Moreover, different tip terminations result in different contrasts for the imaged atomic pattern and, hence, we observe atoms imaged with a disc like shape or as solid rows or with a chain like contrast.

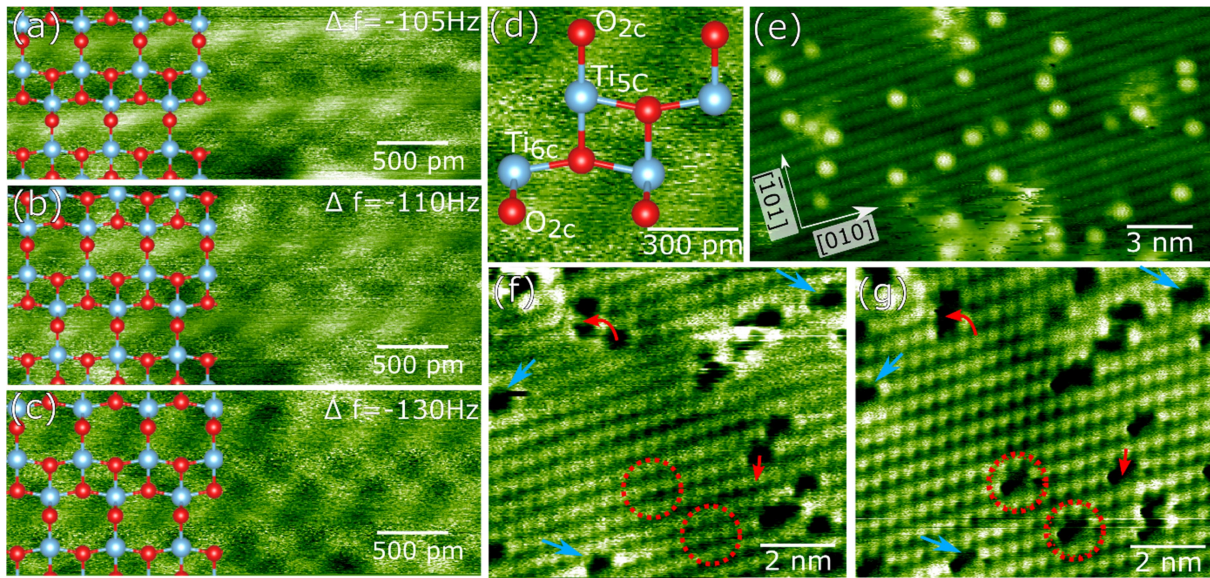


Figure 1. (a-c) Distance-dependent measurements showing contrast transition from O_{2c}-rows to O_{3c}-rows. (e) Imaging mode I showing oxygen rows. (f-g) Imaging mode II showing titanium rows and the mobility of surface defects.