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Structures of $FeTiO_3$ (0001) surfaces observed by scanning tunneling microscopy

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ABSTRACT

Scanning tunneling microscopy (STM) was used to investigate the (0001) surface structure of a natural single crystal of $FeTiO_3$, following argon-ion sputtering and annealing in O_2. Low energy electron diffraction (LEED) of the $FeTiO_3$ (0001) surface shows two different diffraction patterns that depend on preparation. We examined surfaces with a hexagonal pattern that was interpreted as a (1×1) bulk termination. Wide-scale STM images of the (1×1) bulk termination show two distinct co-existing areas: large atomically rough terraces and small, smoother, atomically resolved areas within. The observed single step height of 2.2 ± 0.3 Å (doubled values are also found) plus data from the surface orientation implies that two termination types are seen on the (0001) surface after initial stages of preparation, and that these are either cation-terminated surface planes (Fe^{2+} or Ti^{4+}) or close-packed oxygen terminations. Atomic-resolution STM images of smooth terrace areas show features arranged in a hexagonal array, with a separation of 4.8 ± 0.2 Å. A model is proposed that identifies this termination as an unreconstructed (0001) termination of $FeTiO_3$ that exposes half a layer of either Fe^{2+} or Ti^{4+} cations over a close-packed O layer, with each feature arising from a trimer of O atoms capped by a single cation (Fe^{2+} or Ti^{4+}).