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Unexpected ordering at the atomic scale interface of $SrRuO_3$ and $BaTiO_3$[1]

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Atomically engineered oxide multilayers and superlattices display unique properties responsive to the electronic and atomic structures of the interfaces. Interfaces can exhibit not only two-dimensional functionality, but have the power to dictate the properties of thin films. A clear example is found in ferroelectric thin films, where the domain size, orientation, and transport properties are controlled by top and buried interfaces. We have explored a prototypical ferroelectric - bottom electrode interface by characterizing $BaTiO_3$ grown on $SrRuO_3$. Films were grown on $SrTiO_3$ substrates by pulsed laser deposition, monitored by high-pressure reflection high-energy diffraction, exhibited high crystalline quality in electron diffraction and cross-sectional transmission electron microscopy (STEM), and were flat according to atomic force microscopy. Despite multiple indicators commonly accepted to confirm a sharp interface, atomically the structure is more complex. When grown in a typical oxygen pressure, at or below 10 mTorr, in situ scanning tunneling microscopy (STM) revealed the $SrRuO_3$ surface is littered with oxygen vacancies. For growth or post-annealing above $\sim$100 mtorr, vacancies were removed, but STM and low energy electron diffraction (LEED) disclosed a surface reconstruction consisting of parallel rows with periodicity doubled in one direction. Density function theory (DFT) suggests these rows are chains of Sr and O raised by excess oxygen. Both LEED and cross-sectional STEM revealed that this reconstruction persists at the buried interface and modifies the structure of subsequent $BaTiO_3$ layers. By four layers, the $BaTiO_3$ surface returns to a bulk-like structure with upward polar distortion. This study emphasizes the importance of atomic scale structural studies of what may otherwise appear as sharp interfaces.

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