

Atomic Surface Structures of SrTiO₃ Nanocuboids

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HREM in profile-view mode is an old technique utilized to observe the surface structure of nanoparticles. Marks and Smith first used this technique to successfully resolve the (2×1) reconstruction on the (110) surface of gold nanoparticles in 1983 [1]. However, for the oxide surface, the contrast on the surface is significantly blurred by the delocalization. The implement of aberration correctors can overcome the delocalization problem and help to determine the surface structures on oxide nanoparticles in sub-Å detail. In the present work, we used aberration corrected HREM (Cc and Cs corrected FEI Titan 80-300) to demonstrate the different atomic surface structures on the SrTiO₃ nanocuboids, depending on the synthetic procedures.

SrTiO₃ is one of the most studied materials for its applications in thin film technology and catalysis. SrTiO₃ has a typical perovskite structure, which consists of a repeated stacking of strontium oxide (SrO) and titanium dioxide (TiO₂) layers in the [100] direction. The (100) surface of SrTiO₃ single crystal was found to be SrO, TiO₂ or double-layer TiO₂ reconstructions. SrTiO₃ nanocuboids are mostly (100) surface exposed. However, the atomic surface structures on the SrTiO₃ nanocuboids are unknown. We considered SrTiO₃ nanocuboids synthesized by the oleic acid method [2] and acetic acid method [3]. Both methods were carried out in autoclaves under hydrothermal conditions. For the SrTiO₃ nanocuboids synthesized by the oleic acid method, the surface was SrO terminated with structural relaxation. The surface relaxation also matched with our DFT calculation well. For the nanocuboids synthesized by the acetic acid method, the surface had a multi-domain feature with both SrO and double-layer TiO₂ reconstruction. The mixed termination was expected as the SrO termination and double-layer TiO₂ reconstruction are at the two sides of the lowest-energy surface convex hull [4-5].

References:

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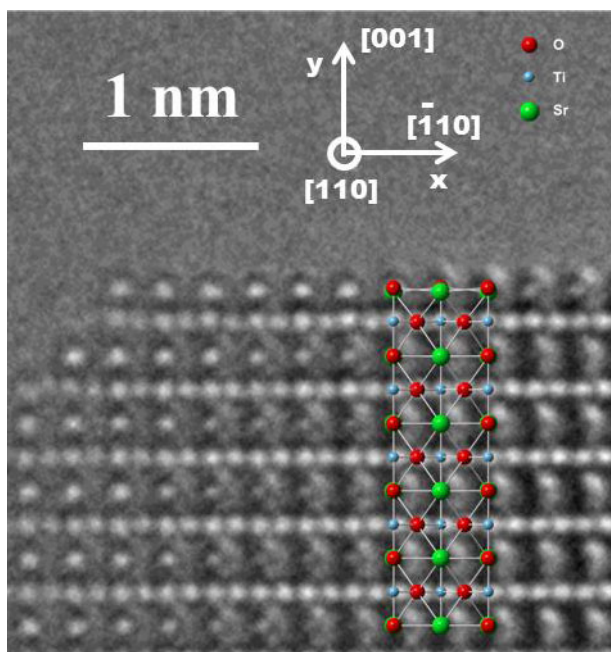


Figure 1. Experimental HREM image of a SrTiO_3 nanocuboid synthesized by the oleic acid method. The surface is SrO terminated with structural relaxation.

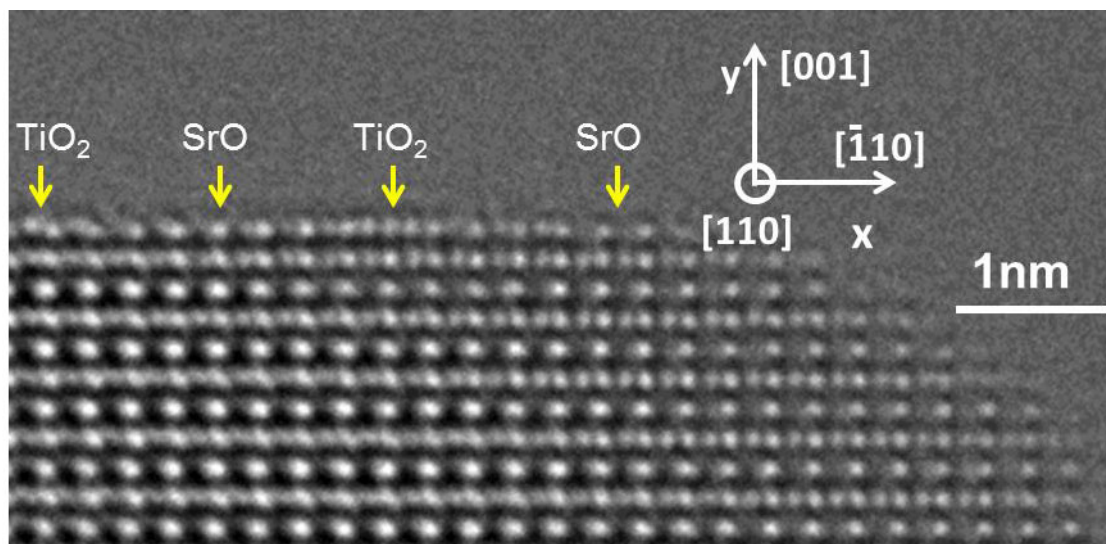


Figure 2. Experimental HREM image of a SrTiO_3 nanocuboid synthesized by the acetic acid method. The surface has both SrO and double-layer TiO_2 reconstructions.