

Abstract Submitted  
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**Structure of Ultrathin Films of Barium Titanate** ERIC COCK-  
AYNE, NIST —  $\text{BaTiO}_3$  is one of the best-known perovskite ferroelectrics, and has  
been extensively studied in its bulk and thin-film forms. Remarkably, a variety of  
new structures (including a dodecagonal quasicrystal) have recently been observed  
in ultrathin Ba-Ti-O films fabricated via various multistep heat treatments of an  
initial thin film perovskite  $\text{BaTiO}_3$  layer deposited on a Pt(111) surface. We have  
found a tiling decoration model for the ultrathin film Ba-Ti-O structures that is fully  
consistent with experimental observations. The structures consist of rumpled Ti-O  
networks with each Ti threefold coordinated with O, and Ba nestled in the larger,  
mainly  $\text{Ti}_7\text{O}_7$ , pores. Simulated STM images show that the circular protrusions  
observed experimentally are the Ba ions. Ab initio molecular dynamics calculations  
demonstrate the stability of our model with respect to competing models for these  
thin film structures.

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