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In situ LEED-IV characterization of polar distorted ultra-thin BaTiO₃ films VON BRAUN NASCIMENTO, E. WARD PLUMMER, University of Tennessee, JUN-SOO SHIN, A.Y. BORISEVICH, ARTHUR P. BADDORF, SERGEI V. KALININ, Oak Ridge National Laboratory — Ferroelectric phase stability in nanoscale ferroelectrics is governed by the interplay of electrostatic depolarization energy, domain formation, adsorption, and surface band bending. Predictions for the minimum critical film thickness for ferroelectricity in BaTiO₃ have continuously decreased with more complex models to a current value of 6 layers. The thinnest experimental value is 12 layers. Using in situ low energy electron diffraction (LEED) I-V, we have characterized the structure of 4 and 10 ML BaTiO₃ films, grown using laser molecular beam epitaxy with fully compressive strain on a SrRuO₃/SrTiO₃ substrate. Analysis of the LEED-IV reveals a surface dead layer with a single-domain upward (out of surface) polarized state below. Intrinsic asymmetry and the stability to compensation of depolarizing charges by dipoles induced by surface stress can explain the single domain scenario. Research was sponsored by the Division of Materials Sciences and Engineering and the Center for Nanophase Materials Sciences, Office of Basic Energy Sciences, U.S. Department of Energy with Oak Ridge National Laboratory, managed and operated by UT-Battelle, LLC.

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