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Interface effect to the nanoscale ferroelectricity CHUN-GANG DUAN, Department of Physics and Astronomy, University of Nebraska, Lincoln, Nebraska, 68588, RENAT F. SABIRIANOV, WAI-NING MEI, Department of Physics, University of Nebraska, Omaha, Nebraska 68182, SITARAM S. JASWAL, EVGENY Y. TSYMBAL, Department of Physics and Astronomy, University of Nebraska, Lincoln, Nebraska 68588 — Recent experimental results demonstrate that in thin films ferroelectricity persists down to film thickness of a few unit cells. This finding opens an avenue for novel electronic devices based on ultrathin ferroelectrics, but also raises questions about factors controlling ferroelectricity and the nature of the ferroelectric state at the nanoscale. Here we report a first-principles study of $KNbO_3$ ferroelectric thin films placed between two metal electrodes, either $SrRuO_3$ or Pt. We show that the bonding at the ferroelectric-metal interface imposes severe constraints on the displacement of atoms, destroying the bulk tetragonal soft mode in thin ferroelectric films. This does not, however, quench local polarization. The critical thickness for the net polarization of the $KNbO_3$ film we found are about 1 nm for Pt and 1.8 nm for $SrRuO_3$ electrodes.

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