

Abstract Submitted
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Surprises in the Growth of SrTiO₃ on Silicon: a Charged Interface and Polar Film. C. STEPHEN HELLBERG, KRISTOPHER E. ANDERSEN, Naval Research Lab — Growth of complex oxides on silicon has been of great interest for device applications. SrTiO₃ has served as the prototypical system, but initial optimism has faded as well ordered epitaxial films have been difficult to achieve. Recently there have been several developments that have dramatically improved our understanding of these systems. Growth of coherent lattice-matched films has finally been achieved, and the measured expansion of the out-of-plane lattice constant exceeds the prediction of the bulk elastic constants of SrTiO₃ by nearly 100%. Simultaneously, growth by a different process in thermodynamic equilibrium yields islands of SrTiO₃. We will present first principles density functional calculations consistent with both experiments: The energetically favored interface is electrically charged, and the film grows ferroelectrically polarized, with an accompanying out-of-plane expansion. Additionally, the films are unstable to phase separation. Methods of substitutionally doping the interface to eliminate the charge are discussed.

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