Abstract Submitted
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Structural stability of highly strained oxide thin films in trilayers YUYANG ZHANG, SOKRATES T. PANTELIDES, Vanderbilt University, and Oak Ridge National Laboratory, TIMOTHY J. PENNYCOOK, University of Oxford , STEPHEN J. PENNYCOOK, Oak Ridge National Laboratory — Thin layers of yttria-stabilized zirconia $(Y_2O_3)_x(ZrO_2)_{1-x}$ (YSZ) sandwiched between $SrTiO_3$ (STO) layers with 7% lattice-mismatch strain are known to have colossal ionic conductivity at room temperature [1]. This phenomenon has been attributed to a disordering of the O sublattice [2, 3]. Here we report first-principle calculations, including checking the existence of negative-frequency phonon modes, that probe the stability of such highly-strained films. We find that, when matched to the STO layers, the strained YSZ cation sublattice remains ordered despite the total disorder of the O sublattice. The disordered anion sublattice will lower the energy of the system and lead to a stable configuration without negative-frequency phonon modes. [1] J. G. Barriocanal et al., Science 321, 676 (2008); [2] T. J. Pennycook et al., Phys.Rev.Lett. 104, 115901 (2010); [3] T. J. Pennycook et al., Eur. Phys. J. Appl. Phys. 54, 33507 (2011).

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