Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Oxygen disorder, a way to accommodate large tensile strains in oxide thin films Y.Y. ZHANG, R. MISHRA, Vanderbilt University, Oak Ridge National Laboratory, T.J. PENNYCOOK, University of Oxford, A.Y. BORISEVICH, Oak Ridge National Laboratory, S.J. PENNYCOOK, University of Tennessee, S.T. PANTELIDES, Vanderbilt University, Oak Ridge National Laboratory — Strain induced by lattice mismatch of epitaxial layers is typically accommodated by misfit dislocations. In transition-metal oxides, other strain-relaxation modes have been observed (oxygen vacancy, octahedral tilts, etc.). Here we use density functional calculations to compare the total energies of different structures and to check for negative-frequency phonon modes, which is an good indicator of instability, and explore the stability of several oxide thin films. We find that when a ZrO2 thin film is sandwiched between SrTiO3 layers (7% biaxial tensile strain), disorder in the oxygen sublattice lowers the energy by 1.4 eV/ZrO2 formula and leads to a stable configuration without negative-frequency phonon modes. Oxygen disorder can also accommodate a 6% biaxial tensile strain in rutile TiO2 thin film. In contrast, we find that if a (LaFeO3)2/(SrFeO3) superlattice is grown on a substrate that imposes an overall biaxial tensile strain, there is a competition between O sublattice disorder, formation and ordering of O vacancies, and octahedral tilts. The mechanism for strain compensation varies with the extent of the strain. We conclude that oxygen-sublattice disorder is one of many ways that tensile strain can be accommodated in transition-metal oxide films.

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Date submitted: 14 Nov 2014

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