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Observations and modeling of defect structures in non-stoichiometric $SrTiO_3$ thin films N. ANTOLIN, R. MISHRA, O.D. RESTREPO, M. DIXIT, R. SRINIVASAN, R. POND, W. WINDL, L. BRILLSON, H. FRASER, The Ohio State University — Z-contrast HRSTEM imaging and EELS has yielded information into the nature of defect formation in thin films of $Sr_{1+\delta}Ti_{1-\delta}O_{3-\delta}$ ($\delta \sim 0.2$) grown on stoichiometric $SrTiO_3$. We envision the creation of regularly spaced anti-phase domains (APD's) separated by anti-phase boundaries (APB's) through a a/2<111> displacement, thus enabling a locally charge-neutral SrO stoichiometry at the APB's, while preserving the $SrTiO_3$ stoichiometry in the interior of the APD's. This allows for an overall charge-neutrality and correct stoichiometry in the non-stoichiometric layer. Preliminary calculations of the dimensions of the APD's are in good agreement with the observed results. We performed molecular dynamics simulations using Buckingham plus Coulomb empirical potentials and their energetics as well as the equilibrium positions of the atoms and resulting lattice constants were determined. Also, the corresponding STEM signals of the structures were modeled, allowing direct comparison to the STEM images of the non-stoichiometric material. To examine the stability of the observed structures in comparison to the constitutional point defects, we calculated the formation energies of single point defects in $SrTiO_3$, which we also used to benchmark the empirical-potential results against first-principles values.

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