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Atomistic simulation of strained $BaTiO_3/SrTiO_3$ superlattices SILVIA TINTE, NIST, MD, MARCELO SEPLIARSKY, IFIR, Argentina, BENJAMIN P. BURTON, NIST, MD — The $BaTiO_3$(BT)/$SrTiO_3$(ST) superlattice is one of the most intensively studied because of the possibility of polarization enhancement by manipulating strain and layer thicknesses. In this work, we apply an atomistic-level description to explore the structural, polar and dielectric properties of epitaxial 001-oriented BT/ST superlattices. The shell-model potentials used here have previously described well the phase diagram and properties of BT perfect crystals and ST in the high-temperature limit, and in combination, these potentials reproduced the FE properties of $Ba_xSr_{1-x}TiO_3$ random solid solutions. Here, we focus on asymmetric BT/ST superlattices with in-plane lattice parameter matched to a ST substrate, and periods ranging from 6 to 18 unit cells. These structures have strain induced tetragonal symmetry at low temperature with polarization along the modulation direction and transform to a paraelectric phase at high temperature. Ferroelectric transition temperatures and static dielectric constant are reported as functions of the BT/ST ratio. Also, we show values for local strain and local spontaneous polarization.

Silvia Tinte
NIST, MD

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