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Strain And Symmetry-induced Structural Transitions in Ultra-thin BiFeO3 Films

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As one of very few room temperature multiferroic materials, bismuth ferrite (BiFeO3: BFO) has been studied extensively in recent years. The bulk form of BFO is known to have a rhombohedrally distorted quasi-cubic perovskite structure with an (a−,a−,a−) octahedral tilt pattern, exhibiting both anti-ferrodistortive displacements and a spontaneous polarization along the <111> axes. Investigating epitaxial thin films under compressive strain, several studies have reported that the polarization direction is tilted towards the [001] out-of-plane direction, while maintaining a significant in-plane component. This effect is accompanied by a significant enhancement of the spontaneous polarization and a series of phase transitions from rhombohedral (R) for small strains to R-like monoclinic (MA) to T-like monoclinic (MC) and to tetragonal (T) for larger strains [1]. Through synchrotron-based 3-dimensional reciprocal space mapping (RSM), facilitated by using X-ray area detectors (Pilatus 100K pixel detector), we have investigated the structure of ultra-thin BFO films grown on SrTiO3 (STO), LaAlO3 (LAO), and TbScO3 (TSO) substrates with thicknesses of only several unit cells. In this thickness regime, the influence of the substrate atomic structure on the properties of the ultra-thin films is very pronounced, and the films exhibit perfect heteroepitaxy up to a critical thickness when the build up of strain energy forces the films into a relaxed structure. Both on STO [2] and LAO, the ultra-thin BFO undergoes a monoclinic to tetragonal phase transition, but with very different c/a axis ratios. On TSO, a very pronounced and well-ordered stripe domainstructure evolves where the domain sizes are strongly thickness- dependent. Argonne National Laboratory's work was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under contract DE-AC02-06CH11357.

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