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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 domain structure 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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