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Symmetry of Highly-Strained BiFeO₃ Films in the Ultrathin Regime¹ YONGSOO YANG, NANCY SENABULYA, ROY CLARKE, University of Michigan, CHRISTIAN M. SCHLEPÜTZ, Argonne National Laboratory, CHRISTIANNE BEEKMAN, WOLTER SIEMONS, HANS M. CHRISTEN, Oak Ridge National Laboratory — At room temperature, highly-strained BiFeO₃ (BFO) films grown on LaAlO₃ substrates exhibit a monoclinic structure with a giant c/a ratio (~ 1.3) when the films are thicker than 4 nm. Their structural symmetry can be controlled by adjusting the temperature [Appl. Phys. Express **4**, 095801 (2011), Adv. Mater. **25**, 5561 (2013)], with a high-temperature tetragonal phase being observed. We report that a structural phase transition can also be achieved by controlling the film thickness: synchrotron x-ray diffraction data shows that the Bragg peak splitting associated with the monoclinic phase disappears as the film thickness decreases below 3 nm, indicating a tetragonal symmetry, but still maintaining the giant c/a ratio. Unlike a similar transition reported for moderately strained BFO grown on SrTiO₃ [APL Mater. **1**, 052102 (2013)], the half-order Bragg peaks indicate that this transition does not involve a significant change in the octahedral tilt pattern of the film. This suggests that the structural evolution of highly-strained BFO films should be understood in terms of the unique (non-octahedral) oxygen coordination of the Fe ion in this highly-strained BFO, not the corner-connectivity of the oxygen octahedra between the film and the substrate.

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