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MS-12-IN-2027 Strain-driven multiferroic thin films and their bi-phase reversibility: a TEM study at atomic resolution

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$BiFeO_3$ (BFO) has been one of the most widely studied multiferroic materials in the past decade. Compared to its bulk crystal with a rhombohedral structure, heteroeptaxially constrained thin film of BFO has demonstrated a significant increase in its intrinsic electric polarization (~60μC/cm^2). The enhancement of the polarization is attributed to its high sensitivity to small changes in lattice structure. Further development in coherent heterostructure of BFO/LAO has therefore put its strain-sensitivitiy into application and successfully produced distortive perovskite structure. pseudo. Pseudo-rhombohedral (R-phase) and super-tetragonal BFO (T-phase) thin films display a high spontaneous polarization up to ~148 μC/cm2. Adding to its outstanding multiferroic behavior the large difference in c/a ratio between R- and T-phase BFO has attracted attention for potential use as energy storage in shape memory device. Although the diversity and multi-functions of BFO phases present an opportunity to implement thin film devices, its stimulus-response and reversibility under harsh conditions remain to be investigated.

In this abstract, we focus on in-situ study of stain-driven BFO thin film where its R-T phase transformation is tuned via strain distribution and temperature control. Focused Ion Beam (FIB) is used to tailor strain distribution at BFO/LAO interface at two dimensions as in-plane epitaxial strain provides driving force for distortive perovskite structures. When the strain is retained in one dimension (LAO//[100]) on purpose and stepped-released along its perpendicular direction (LAO//[010]), interlaced R-T phases are reserved when lamella thickness is above 300nm. Nevertheless, when thickness is reduced down to below ~100nm, only R-phase remains as evidenced by TEM. In addition, it is noticed that the strain-released R-phase presents different lattice structure near the LAO interface. Since ferroic properties are a sensitive function of the relative positions of anions and cations in the structure, HRSTEM is performed to investigate the structure at atomic resolution and with picometer precision. These data can cast light on the interface engineering to alter the polarization.

The reversibility between R-T phases is demonstrated by in-situ TEM. A pure R-phase BFO film at room temperature is transformed into pure T-phase at 400°C in a reversible manner. The c/a ratio difference between T-phase and R-phase gives a maximum full strain of up to ~14% vertical to the thin film interface. As dislocations are crucial to ferroelectric properties including domain walls pinning etc., the possibilities of introducing dislocations during thermal-induced phase transition are studied by in-situ HRSTEM down to an atomic scale.

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