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Domain Structure Control of $BiFeO_3$ Films Through Substrate Symmetry & Film Thickness

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$BiFeO_3$ has attracted great interest owing to their room temperature multiferroic nature with potential applications in spintronic devices and memories. Previous experiments have shown that the ferroelectric domain structure of $BiFeO_3$ films is influenced by strain and the vicinal cut of the substrate. In this work we show the effect of substrate symmetry on the domain structure by examining films grown on low misfit (110) $TbScO_3$, which is a pseudo-cubic perovskite with an orthorhombic distortion.

$BiFeO_3$ films of various thicknesses were grown on (110) $TbScO_3$ single crystal substrates by off-axis radio frequency magnetron sputtering at 690°C. High-resolution x-ray diffraction reciprocal space mapping (RSM) of the films was performed using a four-circle Cu Kα x-ray diffractometer equipped with a four-bounce monochromator. Transmission Electron Microscopy (TEM) was performed using a FEI Tecnai F20, JEOL 2010F, JEOL 3011 and Cs corrected JEOL 2100F. TEM specimens were prepared by mechanical polishing and argon ion milling.

$BiFeO_3$ has a rhombohedral perovskite structure with the polarization along <111> directions. The rhombohedral distortion produces an elongation of the unit cell along the polarization direction which results in four possible ferroelastic variants (Fig. 1a). Normally these 4 variants are degenerate and all four would be expected. RSM mapping and TEM imaging of our $BiFeO_3$ films show that only two ferroelastic domains, r_3 and r_4, are present. Thus the symmetry of the orthorhombic-distorted $TbScO_3$ substrate results in lowering of the energy for the r_3 & r_4 variants and their preferential formation. The domain pattern of the 50 nm $BiFeO_3$ film (Fig. 2) consists of short alternating stripes of the two ferroelastic domains with predominantly vertical domain walls parallel to the $[1\bar{1}10]$ direction. In contrast, the domain pattern of the 400 nm $BiFeO_3$ film (Fig. 3) consists predominantly of alternating stripes of the two ferroelastic domains only along the [001] direction with inclined domain walls. Taking into account domain wall coherency and charge neutrality the vertical boundaries are expected to form between either $r_3^-||r_4^+$, or $r_3^+||r_4^-$ domains and the inclined walls between $r_3^-||r_4^-$, or $r_3^+||r_4^+$ domains[1] (+ or – denotes up or down polarization). In the case of the vertical 109° domain walls the out-of-plane polarization alternates between domains resulting in a zero net polarization (Fig. 1b). Such a structure effectively has no depolarization field and would be expected to form in a film with insulating surfaces (such as $TbScO_3$). The inclined 71° domain walls have a net out-of-plane polarization (Fig. 1c) and if the surfaces are not compensated will result in a depolarization field. However, the 71° domain walls have been reported to be lower in energy[2]. Since the depolarization field increases with decreasing film thickness, it's effect should be more pronounced in the 50 nm film than the 400 nm one.

We conclude that for the thinner $BiFeO_3$ films the depolarization field promotes the formation of a 109° domain pattern and for thicker films the lower energy 71° pattern is favored.

References:
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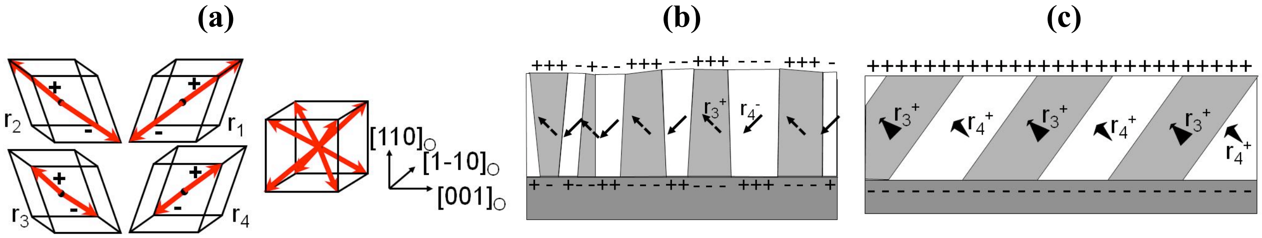

Figure 1. (a) The four ferroelastic variants of $BiFeO_3$ and the two possible polarizations for each. (b) Vertical 109° domain walls and the corresponding out-of-plane polarization. (c) Inclined 71° domain walls and the corresponding out-of-plane polarization.

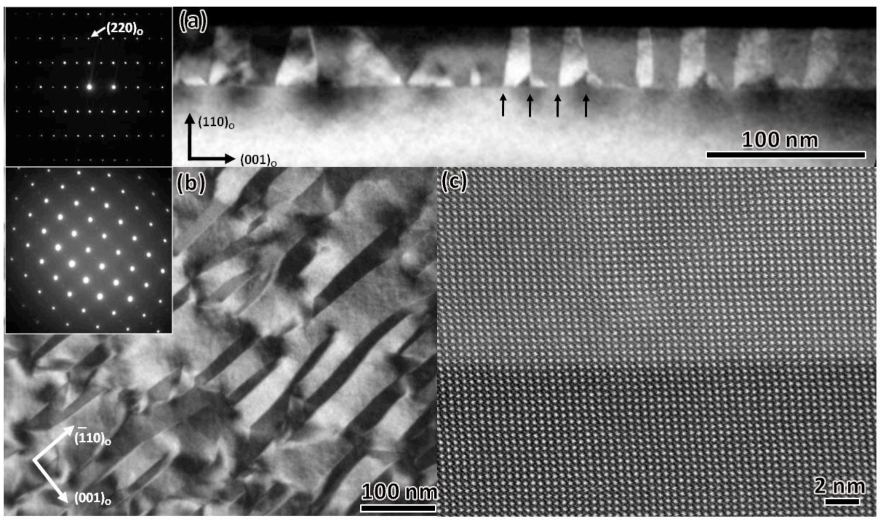

Figure 2. TEM micrographs of 50 nm $BiFeO_3/TbScO_3$. (a) Cross-sectional image showing the 109° vertical domain walls indicated by arrows. Inset shows the diffraction pattern for the film and substrate. (b) Planar view image showing the short striped domain pattern of the film with SAED pattern inset. (c) HAADF STEM image of the $BiFeO_3$ / $TbScO_3$ interface.

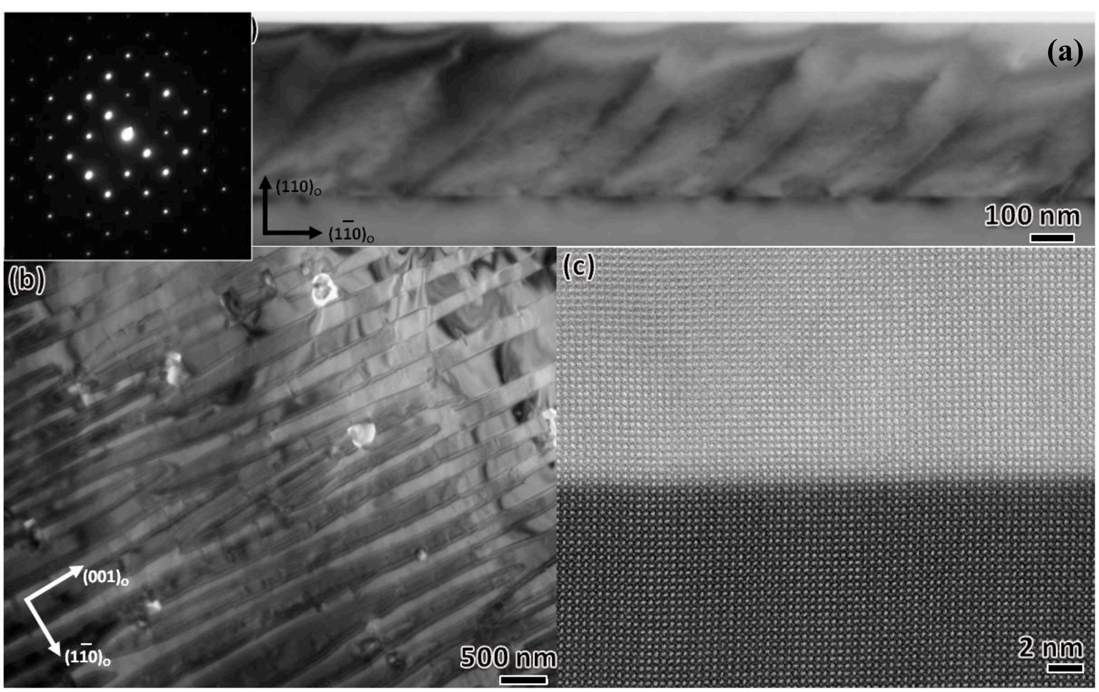

Figure 3. TEM micrographs of 400 nm $BiFeO_3$ / $TbScO_3$: (a) Cross-sectional image showing the vertical domain walls indicated by the arrows. Inset shows the diffraction pattern for the film and substrate. (b) Planar view image showing the striped domain pattern of the film oriented perpendicular to the 50 nm case. (c) HAADF STEM image of the $BiFeO_3$ / $TbScO_3$ interface.

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