Enhanced Multiferroic Properties by Stress Modulation in $Ba(Cu_{1/3}Nb_{2/3})O_3$-doped Epitaxial $BiFeO_3$ Thin Film

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As domain walls have a completely different polarization configuration from that of interior domains in ferroelectrics, investigations of their physical properties, including the thickness, conductance, and variations in atomic displacement, have been central issues to understand the correlation between overall ferroelectric behavior and dynamics of polarization switching [1]. In addition to the traditional Bloch-type domain walls in ferromagnetics and the Ising-type domain walls in ferroelectrics, notable experimental studies recently demonstrated that peculiar types of domains and their walls [2,3], such as nanoscale rotational vortices [4,5] and antiparallel dipole configurations [2,3], could appear in ferroelectric oxides films. By using a combination of high-angle annular dark-field scanning transmission electron microscopy (HAADF-STEM), geometric phase analysis (GPA), and density functional theory (DFT) calculations, here we show that, in epitaxial $BiFeO_3$ films at atomic resolution as shown in figure 1, large out-of-plane coherent strain without any misfit dislocations or precipitations can be locally induced inside the films through chemical modification and subsequently head-to-head and tail-to-tail domain walls that are usually considered to be energetically unfavorable form with different wall thickness (figure 2). The present study thus reveals that local variation in strain field has a substantial impact on the formation of unusual domain wall structures in $BiFeO_3$, suggesting plausible flexoelectricity by proper doping.

References

[1] G. Catalan, Reviews of modern physics 84 (2012) 119
[2] G. Catalan et al., Phy. Rev. Lett. 96 (2006) 127602
[3] C.-L. Jia et al., Nat. Mater 7 (2008) 57
[4] A. Schilling et al., Nano Lett. 9 (2009) 3359
[5] C. T. Nelson et al., Nano Lett. 11 (2011) 828

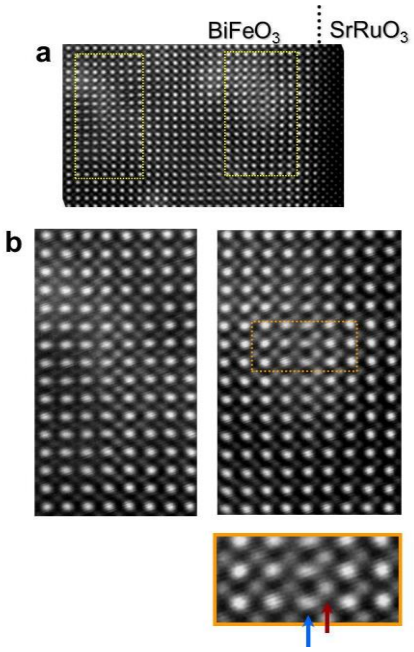

FIG. 1. HAADF-STEM images of 10%-Ba($Cu_{1/3}Nb_{2/3}$)O_3-doped $BiFeO_3$ films on $SrRuO_3$ bottom electrode layers. (a) An overview Z-contrast image confirming the epitaxial growth of the films. (b) Magnified images for the regions denoted by yellow rectangles in (a). The enlargement shown at the bottom for the region denoted by an orange rectangle is provided to clarify the different contrast features at both Bi and Fe columns, as indicated by blue and red arrows.

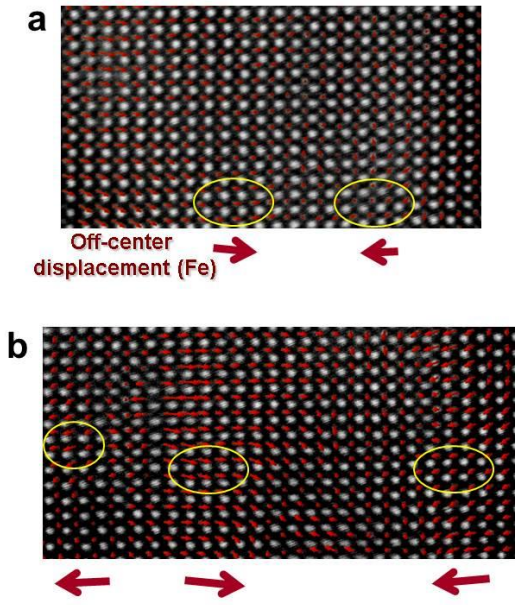

FIG. 2. Plots of off-center Fe displacement vectors. (a) Low-strain region. (b) High-strain region. The displacement vectors are superimposed on each STEM image, showing much larger magnitudes in the high-strain region. For direct comparison and better visualization, thick red arrows are included to represent the direction of the Fe displacement vectors in the domains denoted by yellow ovals. Antipaarllel polarizations of the dipoles between domains are noted.