ADVANCED MATERIALS

Supporting Information

for *Adv. Mater.*, DOI: 10.1002/adma.201400557

Electronic Properties of Isosymmetric Phase Boundaries in Highly Strained Ca-Doped $BiFeO_3$

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Supplementary Information

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Reciprocal space maps (RSMs) of the 001 (LAO)-diffraction condition of the BFO thin films with 2% Ca doping are shown in Fig. S1 a). The 001 diffraction peak of the substrate and the characteristic R and T phase peaks are visible. No significant difference has been observed in the lattice parameter measurement between doped and undoped thin films. The R phase out-of-plane lattice parameter is c = 4.17 Å. A detailed analysis of the RSM reveals the existence of satellites peaks on either side of the R and T phase diffraction peaks corresponding to a phase tilt of 1.53° and 2.88° that can be correlated to the topography of the films [1]. RSM performed at the (103) reflection are shown in Fig. S1 b) and c). Combined with the (001) RSM this allowed us to estimate the in-plane lattice parameter of the strained R-phase to be 3.82 Å revealing the high strain imposed to the film.

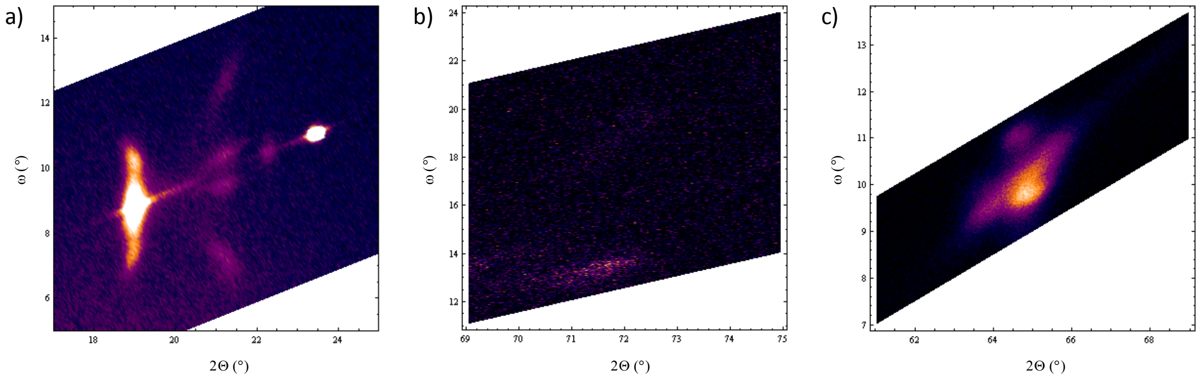

Fig. S1 RSM of the 001-diffraction peak (a) and 103-diffraction peak (b and c) of the BFO thin films with 2% Ca doping.

In order to acquire deeper insight into the structure-conductivity relation, we performed combined HAADF-STEM and EELS studies of the structural phases and boundaries (Fig. 3 in the main manuscript). HAADF images were obtained from a spherical aberration-corrected microscope (TEAM0.5). The raw EELS data is shown in figure S2.

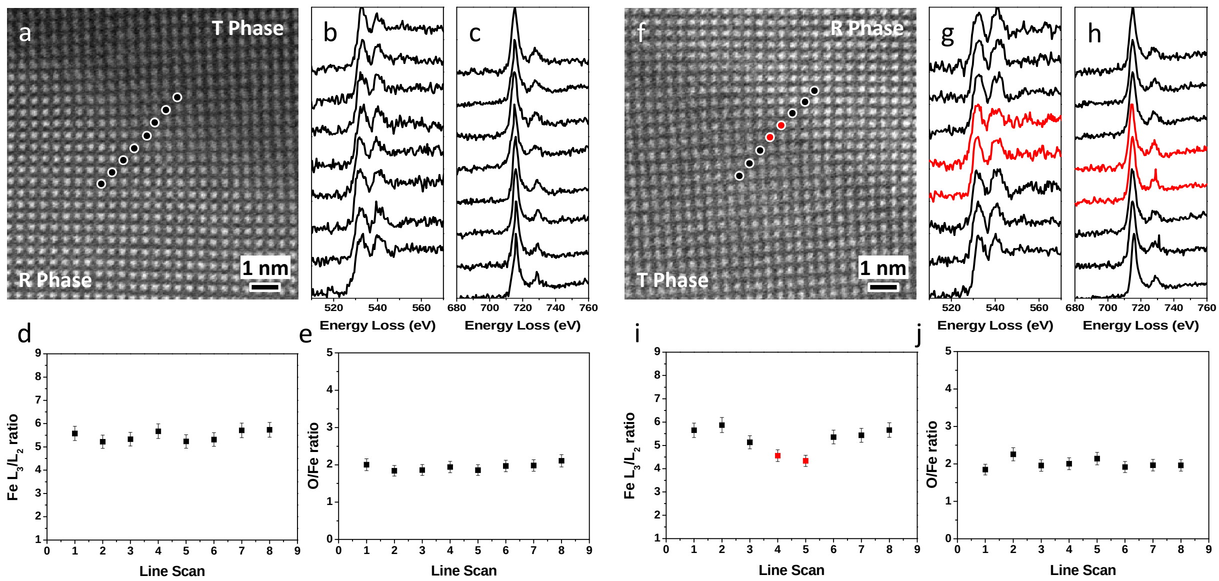

Fig. S2 a) HAADF image of soft R-T boundary and local EELS spectra for O-Kedge (b) and Fe-L edges (c) across the boundary. d) and e) Fe L3/L2 and O/Fe signal ratio. f) HAADF image of sharp R-T boundary and local EELS spectra for O-Kedge (g) and Fe-L edges (h) across the boundary. i) and j) Fe L3/L2 and O/Fe signal ratio.

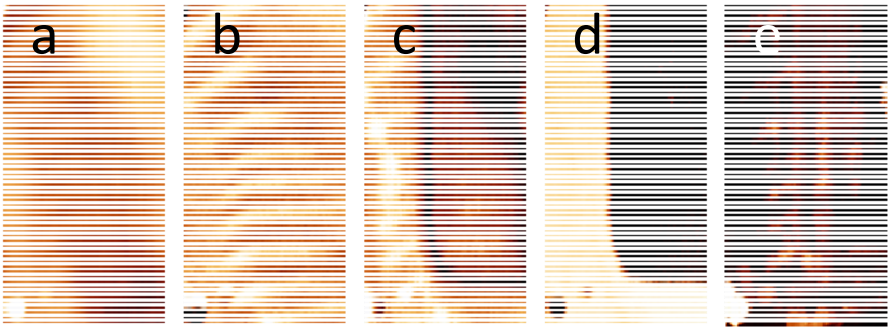

Fig. S3 Domain boundary conductivity for reversed out-of-plane polarization. a) topography, b) deflection signal, c) out-of-plane PFM amplitude, d) out-of-plane PFM phase, e) c-AFM.

Fig. S3 shows experimental scanning probe results on regions where the out-of-plane polarization is reversed by poling with a biased AFM tip (dark area in d). The locations of "soft" and "sharp" phase boundaries do not depend on the out-of-plane polarization direction, i.e. compare topography, deflection with piezoresponse (PFM) phase. Higher electronic conduction is seen at phase boundaries with both out-of-plane ferroelectric orientations.

References

[1] Damodaran, A. R., et al., Nanoscale Structure and Mechanism for Enhanced Electromechanical Response of Highly Strained $BiFeO_3$Thin Films, Adv. Mat. 23, 3170 (2011)