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Monitoring Bismuth Ferrite Domain Walls Behavior Under Electric Field With Atomic Resolution By *In Situ* Scanning Transmission Electron Microscopy

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Two dimensional interfaces between ferroelectric domains with distinct polarization vector orientation are called the domain walls (DWs). Since the early exploration of ferroelectricity, it has been stated in a simplistic manner that DWs are compelled to move when an external electric field is applied as a consequence of polarization switching. DWs electronics is a relatively new concept that aims at taking advantage of the electric-field-controlled DW movement and integrate it into nano-level (or even atomic-level) devices. Crucial to the realization of DWs electronics, it is to understand the fundamentals and complexity of polarization switching and DWs' dynamics at relevant local scales, e.g the atomic scale. This has recently become possible thanks to the development of high-resolution voltage bias *in situ* techniques [1].

In the present work, we analyze the interaction between the electric field and DWs in ferroelectric $BiFeO_3$ (BFO) single crystal at the atomic scale using *in situ* scanning transmission electron microscopy (STEM). The specimen is prepared in a parallel plate capacitor configuration (Figure 1) on dedicated chips with patterned electrodes processed by focused ion beam (FIB) with gallium ion source. The capacitor-like device has the advantage of creating homogeneous electric field compared to other TEM voltage bias *in situ* techniques configurations, such as probe techniques [2-3]. While sample preparation with FIB can be challenging, targeting atomic resolution makes it particularly meticulous. High quality atomic resolution images require a specimen thickness of less than 100 nm, but at the same time the mechanical stability of the device must be maintained; therefore, additional details on specimen preparation will be discussed.

The domain structure of BFO single crystal was previously determined using atomic resolution TEM [4] and consists of lamellar features of ferroelastic DWs and purely ferroelectric (180˚) zigzag DWs. To the best of our knowledge, no considerations about the dynamics of DWs in BFO single crystal has been previously reported. Herein, we investigate how the zigzag DWs respond to externally applied voltage. Information about the polarization vector is indirectly retrieved from the Fe-displacement in respect to the center of the Bi-sublattice map evaluated from High Angle Annular Dark Field (HAADF) [5]; Fe-displacement is proportional but points in opposite direction to the polarization vector.
We directly monitor with atomic resolution the switching of polarization and movement of the midsection of an individual zigzag DWs (Figure 2). One limitation of the STEM technique is that we access only a 2D view, projected along the electron beam. In the presentation we will discuss the possible 3D switching paths of the polarization vector taking into account the interplay between the

direction of the electric field, the 3D configuration of the polarization in rhombohedral structure of BFO and previous literature studies. Further, we show that the tip of the zigzag DWs interacts differently with the electric field. In contrast with the midsection which is uncharged, the apex of the wall is negatively "tail-to-tail" charged. Our results show that when electric bias is applied, on one hand, the apex is changing the curvature and on the other hand, the Fe-displacement vector magnitude and orientation change in the vicinity of the wall. As a result, the bound charge distribution at the apex of the zigzag DWs changes.

The present work aims at a fundamental understanding of the emergent phenomena describing the interaction of DWs with the electric field. We show, down to the atomic level, that the interaction is complex involving DW motion, change in the DW plane, modification of the unit cell distortion and strain re-distribution. [6]

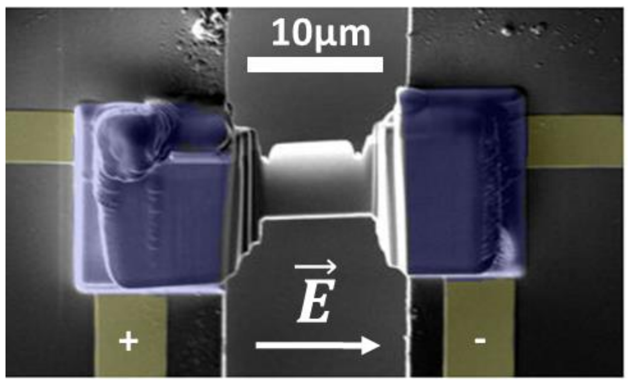

Figure 1. False color scanning electron microscopy image of BFO single crystal specimen mounted on the voltage biasing chip in a capacitor-like configuration. The Pt deposited (marked in blue) has the role of welding the specimen on the chip but also assuring electrical contacts with the chip patterned electrodes (marked in yellow)

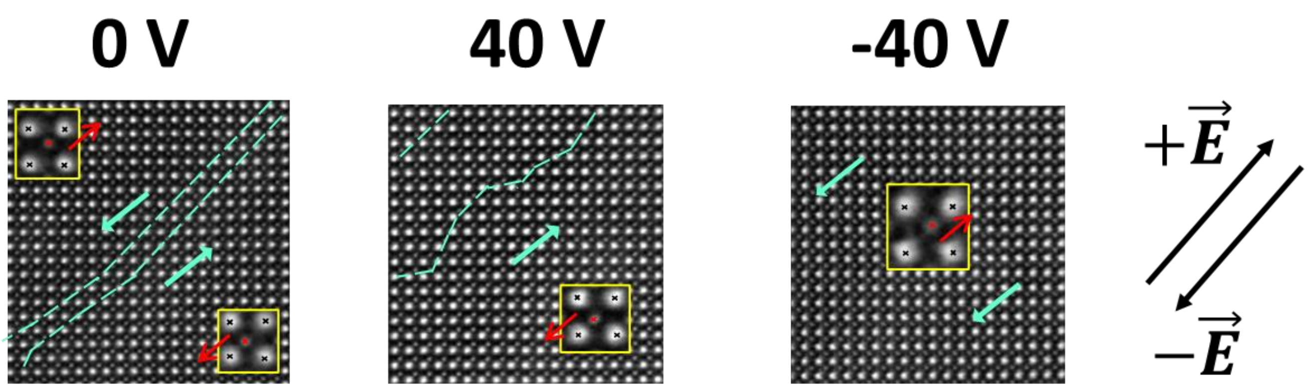

Figure 2. HAADF-STEM image of a DW region in BFO single crystal at 0 V, 40 V and -40 V, respectively. The DW region is marked with dotted blue line. Note that at -40 V the DW was completely moved away from the analyzed area. The Fe-displacement vector in respect with the Bi-sublattice is marked with red arrow while the direction of the polarization vector is indicated by blue arrow. The direction of the electric field is indicated with black arrows. The scale bar is 2 nm.

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