Atomic-Scale Structural and Chemical Analysis of Domain Walls In Bismuth Ferrite

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Ferroelectric bismuth ferrite has been extensively studied as a candidate material for high-temperature piezoelectric devices. One of the drawbacks of this material is its high electrical conductivity which often stems from the local conduction at the domain walls [1,2,3]. Mobile charged defects, accumulated at the domain walls to screen polarization charges, have been proposed in several ferroelectrics as the origin of this local conduction, however, the presence of defects has not yet been directly confirmed.

In order to make further steps toward the understanding of the domain wall conductivity, we investigated the local structure of domain walls using state-of-the-art aberration corrected electron microscopy. In the talk, a direct evidence of the accumulation of charged defects at domain walls in bismuth ferrite using chemical and structural analysis on the atomic scale will be presented and discussed. We elaborated two analytical methods (electron-energy loss spectroscopy and quantitative high-angle annular dark-field imaging) allowing chemical analysis at the atomic scale, which lead to the identification of iron (IV) ions and bismuth vacancies accumulated at the domain walls. Iron (IV) ions in bismuth ferrite are associated with electron holes, thus leading to p-type hopping conduction at the domain walls. [4] We will further discuss the domain wall mobility studied by ex-situ poling experiments. Finally, we will show that the local domain-wall conductivity can be tailored by material processing. The results open up possibilities for engineering local conductivity in ferroelectrics by fine control of the type and concentration of point defects.

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