Effect of single point defect on local properties in $BiFeO_3$ thin film

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Ferroelectric materials have a promising future in non-volatile memories and high-density information storage. Most of these applications require stabilization of the switch process and it depends on the move of domain wall. Defects also act as pinning centers that usually prevent the motion of domain wall, as a result, the existence and influence of defect is of great interest in both fundamental and practical research. It has been confirmed that different kinds of defects have different impact on film properties and there are a lot of defects has been studied experiment and theory until now. Single point defect has been observed and it has an important influence on the move of domain wall, but the effect of single point defect on local properties is not fully studied.

We combine high resolution scanning transmission electron microscopy(STEM), high-angle annular dark field(HAADF) imaging and geometry model based on density functional theory to study the influence of local point defect in an epitaxial bilayer of an antiferromagnetic ferroelectric ($BiFeO_3$) on a ferromagnetic electrode($La_{0.7}Sr_{0.3}MnO_3$). We utilize STEM to directly determine the position of each atom. This allows us to directly determine the element, polarization, lattice constant on atomic level. We combine experiment results with atom configurations which based on density functional theory together to simulate the crystal structure in the specific area and its STEM image, this allows us to acquire some quantitative information. From the one-to-one correspondence between the experimental and theoretical, we observed localized point defect of heavy-element Bi atoms substitution in the Fe sites in $BiFeO_3$ thin film, and the polarization of the region adjacent to the point defect is decreased by more than 30 percent. And the point defect may act as an active pinning site during the polarization switching process. We think that the point defect could pin the domain wall, and it is probably the reason for the fatigue of ferroelectric material.

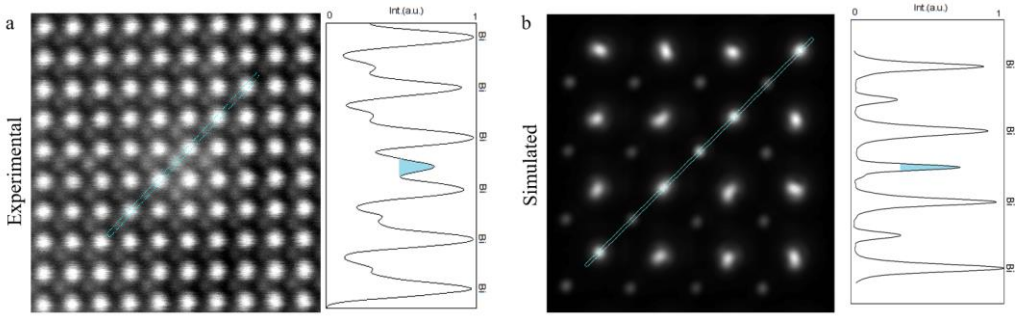

FIG.1. The heavy-element Bi substitution in the Fe site. (a) Experimental HAADF-STEM image of the area with point defect in the 50nm thick epitaxial $BiFeO_3$ thin films with 20nm $La_{0.7}Sr_{0.3}MnO_3$ buffered electrodes. The right line intensity profile corresponding to the dashed blue line, the blue peak in right image is the point defect intensity. (b)Simulated HAADF-STEM image of the area that Bi substitution in the Fe site partly. This image with the corresponding simulated line intensity profile is compared with the experimental image.

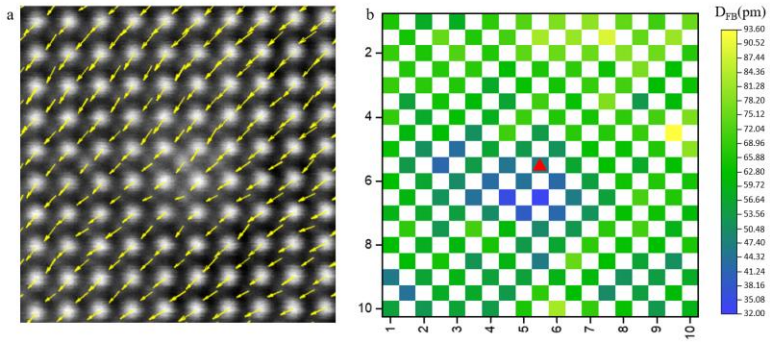

FIG.2. Polarization map of the point defect region. (a)The same HAADF STEM image as Fig.1a overlaid with the polarization vectors. From this map it is apparent that the polarization direction is accordance in this region, but the magnitude around the point defect become smaller. (b)the corresponding 2D quantify displacement map of the bismuth and iron atoms. Every colorful foursquare parallelism an atom in the left image. The red triangle highlights the location of point defect.

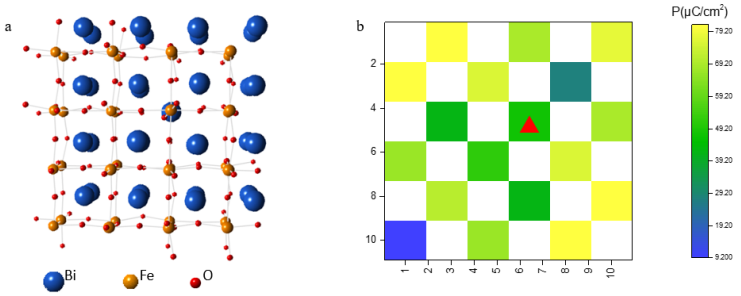

FIG.3 Simulated polarization map. (a) The schematic of the heavy-element Bi atom substitution in the Fe atom site. (b)The corresponding 2D quantify displacement map of the bismuth and iron atoms.

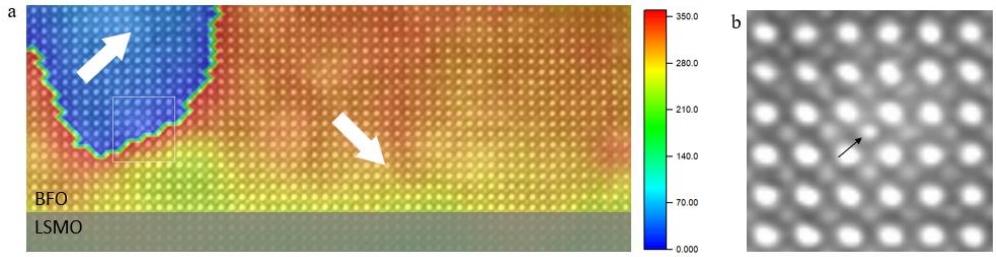

FIG.4 A point defect beside the 109°domain wall, with corresponding color maps of the angle of polarization. (a)A HAADF image of a region containing a point defect and 109° domain wall in the 10nm thick epitaxial $BiFeO_3$ thin films with 20nm $La_{0.7}Sr_{0.3}MnO_3$ buffered electrodes. The white arrows in the image represent the polarization direction. (b) The HAADF image shows the point defect corresponding to the region of white frame in the FIG.4(a), the black arrow shows the point defect.

Acknowledgements

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