**Interface effects on the epitaxial growth characteristics of brownmillerite $SrFeO_{2.5}$ thin film grown on $SrRuO_3$ and $SrTiO_3$**

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The rich properties and broad utility of transition metal oxides are enabled by the strong coupling among the lattice, charge, spin, and orbital degree of freedom, which basically originates from the strong hybridization between transition metal d and oxygen 2p orbitals [1,2]. Engineering such complex correlations has thus been recognized as a route for tailoring functional properties of transition metal oxides. In recent years, unprecedented physical phenomena further emerged by manipulating the heterointerface of transition metal oxides, such as two-dimensional free electron gases, interface charge transfer, high-Tc superconductor, and colossal magneto resistance, which have never been accessed in their bulk equilibrium phases [3]. These new phenomena were born through the interface effects determined by, for instance, structural distortions, crystal chemistry, and oxygen coordination environments of the heterointerface between different oxides, which essentially modifies the degree of the orbital hybridization.

The interface effects could also exert a great influence on the growth dynamics of oxide thin films on foreign substrates. Traditionally, the epitaxial strain caused by lattice mismatch with substrates has been widely employed to manipulate the growth process of the thin films. However, it is rather complex and limited to control the growth process of the thin films by imposing the epitaxial strain alone. Various interface effects can extend the range of choice, but they were rarely reported despite their great importance and potential for manipulating the growth dynamics and consequential physical properties of oxide thin films. Totally different growth behavior of oxide thin films would happen depending on the heterointerface structures, including their crystal symmetry, orientation, and oxygen coordination environments. Therefore, characterizing the microstructures of the oxide heterointerface is quite important for understanding how the interface effects influence the growth characteristics of oxide thin films and for fabricating the functional devices having desired physical properties.

Here, we report that the interface effects can play a crucial role in controlling the growth behavior of oxide thin films by overriding the simple epitaxial strain effect. To verify such interface effects, microstructures of BM-SFO thin films grown on STO(001) and SRO/STO(001) substrates were observed at the atomic scale using scanning transmission electron microscopy. The BM-SFO thin films showed multi-domain structures on the abrupt interface with SRO/STO(001) whereas *b*-axis oriented growth was revealed on the transition layer formed between BM-SFO and STO(001) (Fig. 1). The growth behavior of BM-SFO/STO(001) predicted by the first-principles calculations, *i.e. a*-axis oriented growth, was also different from that displayed in Fig. 1d - f (Fig. 2). This is attributed to the formation of perovskite-like SFO transition layer at the interface which acts as a buffer layer for the BM-SFO growth (Fig. 3). These discrepancies in the growth processes of the thin films were found to originate from the interface effects influenced by the growth condition as well as the different chemical species at the interface. These results are expected to be valuable for controlling the direction of the oxygen vacancy channel, which has been a hot issue in a wide range of scientific and industrial areas.


[1] Goodenough J.B. *et al. Rep. Prog. Phys.* **67,** 1915 (2004)

[2] Zubko P. *et al. Annu. Rev. Condens. Matter Phys.* **2,** 141 (2011)

[3] Ohtomo A. *et al. Nature*, **427,** 423 (2004)


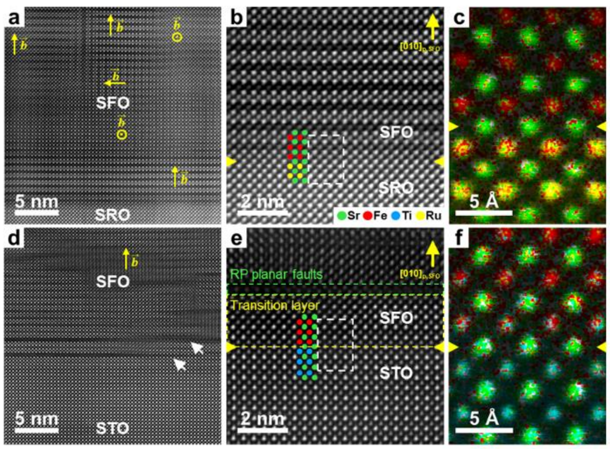


Figure 1. Atomic configurations of BM-SFO thin films at the interface. (a,d) Cross-sectional HAADF-STEM images of (a) BM-SFO/SRO/STO(001) and (d) BM-SFO/STO(001) at the interfaces. (b,e) Magnified atomic-resolution images of a and d at the interfaces, respectively. (c,f) Atomic-resolution EDS elemental maps at the interfaces from the regions marked by white-dashed rectangles in b and e, respectively.

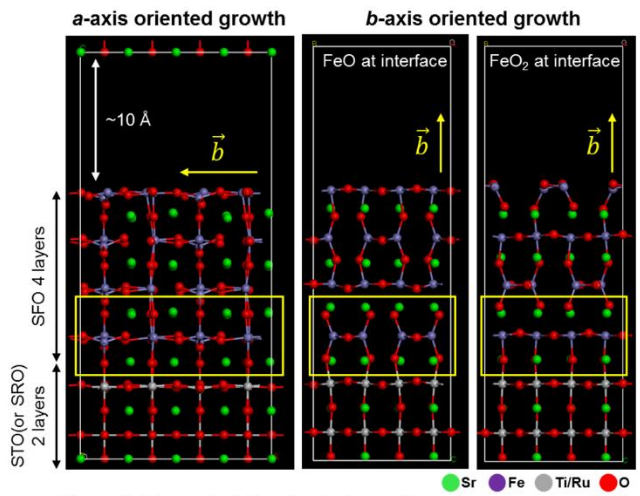


Figure 2. First-principles simulations of atomic structures at BM-SFO/STO(001) and BM-SFO/SRO(001) interfaces. Four layers of BM-SFO with growth directions of *a*- and *b*-axis are placed on two layers of STO and SRO, respectively. For *b*-axis growth, two different interface structures having FeO and $FeO_2$ layers at the interface are calculated.

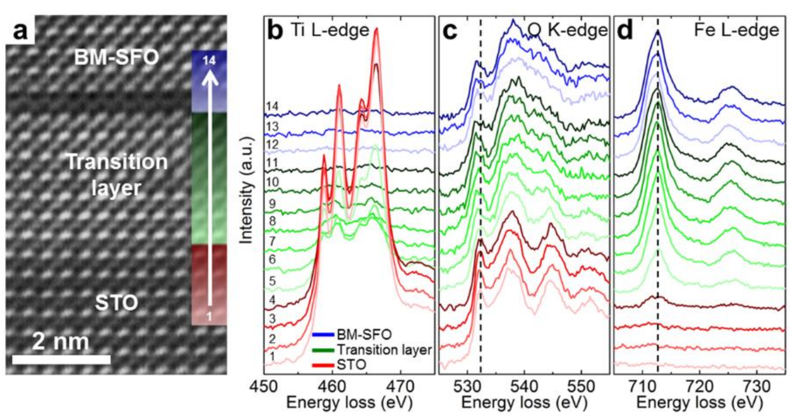


Figure 3. Identification of transition layer using EELS measurements. (a) HAADF-STEM images of BM-SFO/STO(001) at the interface. (b–d) A series of ELNES at (b) Ti $L_{2,3}$-edge, (c) O K-edge, and (d) Fe $L_{2,3}$-edge. These spectra were acquired across the heterointerface from the STO substrate through the transition layer to the BM-SFO thin film, marked in red, green, and blue, respectively, at the corresponding regions in a.