## Highlights

Innovative materials with strong interplay of spin orbital charge and topological degrees of freedom - 2018

## Designing antiphase boundaries by atomic control of heterointerfaces

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Surface-type defects are known to influence the achievement of desired material performance. Therefore, a strategy to design and manipulate defect nucleation and formation can improve our understanding and in principle lead to the ability to control performance. The focus of this paper is the design of 2D surface-type defects, such as antiphase boundaries (APB). The origin of antiphase domains (APDs) in La<sub>2/3</sub>Sr<sub>1/3</sub>MnO<sub>3</sub> (LSMO113) thin film grown on Sr<sub>2</sub>RuO<sub>4</sub> (SRO214) substrate is explored via the combination of advanced growth, atomic-resolved electron microscopy, first-principles calculations and defect theory. We observed that APBs in the La<sub>2/3</sub>Sr<sub>1/3</sub>MnO<sub>3</sub> film naturally nucleate at the step on the substrate/film (SRO214/LSMO113) interface (Fig. 1 and 2). Furthermore, atomic-resolved electron microscopy investigation showed that these APBs tend to merge when two steps exist at short distance to minimize the APB surface energy (Fig. 2). Such a design philosophy can be easily transferrable to many oxide-based heterostructure system as well as providing new aspects in non oxide wafers.

Fig. 1: HAADF-STEM image of LSMO113/SRO214 taken along the [100] direction, showing nucleation of APB at the step on the SRO214 substrate surface. The yellow lines indicate the interface where SRO substrate terminates with the SrO layer. The structural model is overlaid across the APB. The APB parallel to the (100) plane with double AO layers is marked by the vertical red line. The SRO unit cell is shown at the bottom left.





Fig. 2: The triangular APDs in the LSMO film on the SRO214 substrate with steps. Atomic-resolved HAADF-STEM images of a triangular APD taken along the [100] direction. The substrates are marked in blue and films in purple to emphasize the step position. The antiphase boundaries are indicated with yellow dotted lines. The LSMO region grown on the lower part of the step is defined as APD-L, and the higher part as APD-H.



