Interfacial Structure in Epitaxial Perovskite Oxides on (001) Ge Crystal

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Abstract

Perovskite oxides films have attracted much attention due to their intriguing electrical, magnetic, and optical properties. In the hetero-epitaxial thin film system, as the film grows up to a certain thickness, interfacial dislocations are expected to form to relax the strain. Intensive transmission electron microscopy (TEM) work has been performed for perovskite-on-perovskite systems, e.g., PZT/$SrTiO_3$,[1] $SrTiO_3$/$LaAlO_3$,[2] *et al*. It is well recognized that the interfacial dislocations are crucial for some physical properties of the thin film.[3,4] Very recently, high-quality epitaxial perovskite thin films on semiconductor wafers have been achieved. However the nature of interfacial dislocations in this perovskite-on-diamond system has never been reported.

We investigated the interfacial structure of perovskite ($SrZr_{0.68}Ti_{0.32}O_3$, SZTO) thin film on (001) Ge single crystal, using various TEM techniques. In contrast to the most found dislocations with Burgers vectors of $\boldsymbol{a}$ <100> in perovskite heterostructures (cubic-on-cubic system), we observed dislocation-loop with a Burgers vector of ½$\boldsymbol{a}$ <111>. We also found the dislocation reaction from two partial dislocations to one perfect dislocation $\frac{1}{2}\boldsymbol{a}\,[1\bar{1}1] + \frac{1}{2}\boldsymbol{a}\,[11\bar{1}] = \boldsymbol{a}\,[100]$, which leads to the formation of threading dislocation with Burgers vector of $\boldsymbol{a}$ [100]. In addition, we found the coupling of dislocation half-loop with anti-phase boundary (APB, shift vector of ½$\boldsymbol{a}$ <111>) induced by lattice terrace of Ge and they can decouple after annealing. The possible models based on the half-loop theory are also proposed for the dislocation reactions and the coupling behavior.

Our findings on the interfacial dislocations, which are for the first time reported in perovskite-on-diamond system, describe the nature of the interface between semiconductors and perovskite, and give valuable insights on how the misfit strain is relaxed. It will help the researchers who investigate and develop the semiconductor-based functional oxide devices, to optimize their design and growth techniques.

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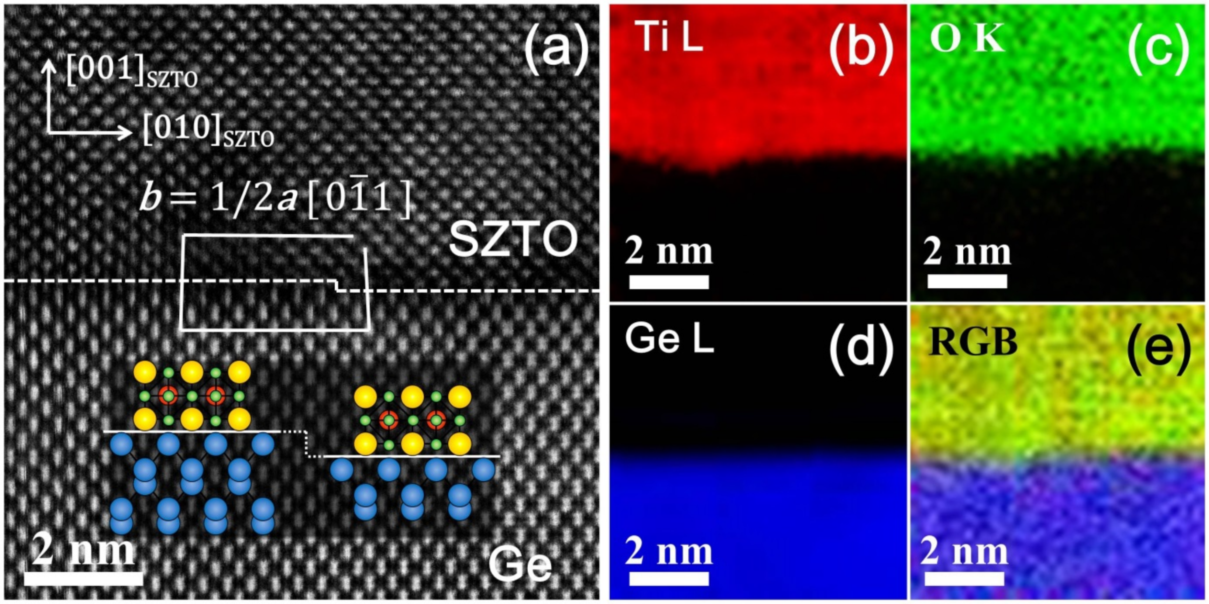

Figure 1. (a) Cross-sectional STEM image with Burgers vector along $[0\bar{1}1]$ direction. The Burgers circuit is drawn around the dislocation core. Schematic diagram of step and terrace structure is shown in the inset. Elemental maps (50 pixels by 50 pixels) from STEM EELS of Ti (red), O (green), Ge (blue) and their RGB mixture are shown in (b), (c), (d), and (e), respectively.

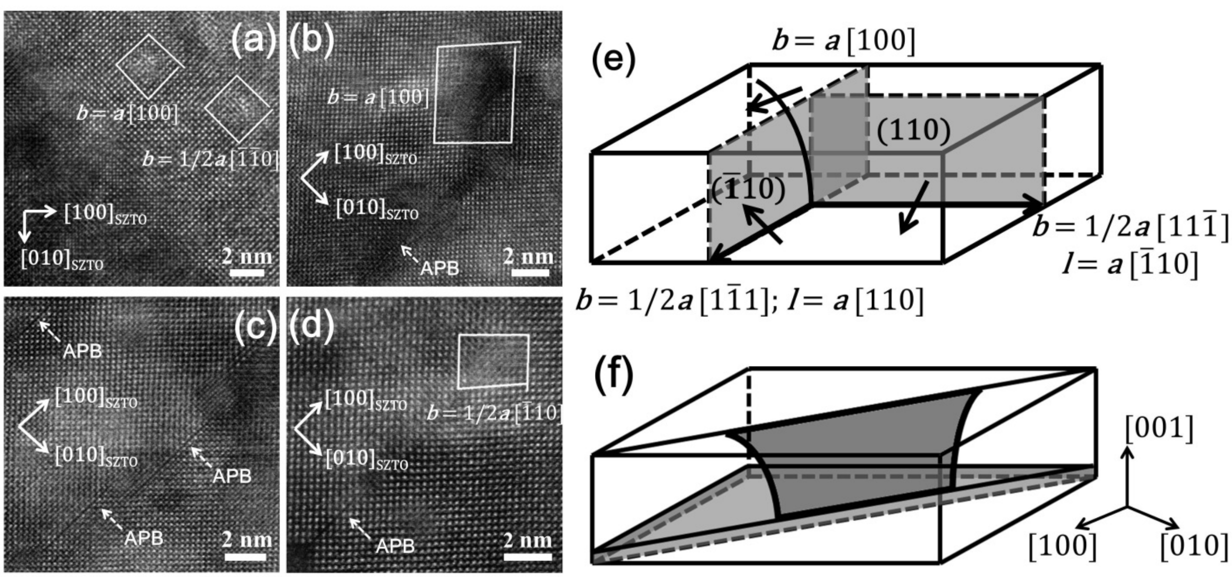

Figure 2. (a) Plane-view HRTEM image of SZTO thin films. HR-STEM images of the plane view are shown in (b), (c), and (d). The APBs are indicated by white dashed arrows. Schematic diagrams of dislocation dissociation and coupling behavior between APBs and dislocations are shown in (e) and (f), respectively.