New Line Defect in Epitaxial $BaSnO_3$

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Defects are present in all real crystals and they modify the properties of materials. By virtue of advancement in electron microscopy, visualization of not only predicted defects but also new kinds of defects is now possible [1-3]. A recent discovery of a new line defect in $NdTiO_3$ hinted at the presence of more diversified line defects in perovskite materials [3]. Here, we report a unique line defect observed in a perovskite $BaSnO_3$ thin film. Compositionally and structurally different from the host $BaSnO_3$ perovskite crystal, this line defect is aligned along the film growth direction and shows an atypical atomic configuration.

A DC sputter deposition method was used to grow 200 nm-thick La-doped $BaSnO_3$ thin films on a $LaAlO_3$ substrate [4]. Subsequently, scanning transmission electron microscopy (STEM) experiments were carried out using an FEI Titan G2 60-300 (S)TEM at 200 keV. The energy dispersive X-ray spectroscopy (EDX) spectra and elemental maps were acquired using the FEI Super-X EDX detector and electron energy-loss spectroscopy (EELS) spectra were measured using the Gatan Enfinium ER spectrometer.

Fig. 1(a) shows a plan-view high-angle annular dark-field (HAADF) STEM image of the $BaSnO_3$ film. The line defect can be seen (highlighted in a boxed area) in addition to typical edge dislocations. Strong strain contrast around these defects is also observed in a low-angle annular dark-field (LAADF) STEM image from the same region (see Fig. 1(b)). A STEM-EDX elemental map of the line defect is shown in Fig. 2. The elemental map reveals that two Ba columns are missing and two Sn columns are rotated 90° degree from their original positions around the line defect core. Consequentially, the chemical bonding and electronic structures of the core is expected to be different from a perfect crystal. Utilizing EELS and density functional theory-based calculations, we explore the electronic structure (the band gap, density of states, effective masses of charge carriers, etc.) of this line defect. In addition, its connection with a coexisting 2-D defect, Ruddlesden-Popper faults, is discussed.

Beyond demonstration of this unique 1-D defect in perovskite epitaxial films, this study raises more questions about conditions creating these peculiar defects, their effects on the materials' overall electronic and magnetic properties, and their properties that possibly can be utilized by defect engineering, which needs to be further investigated in the future [5].

Reference

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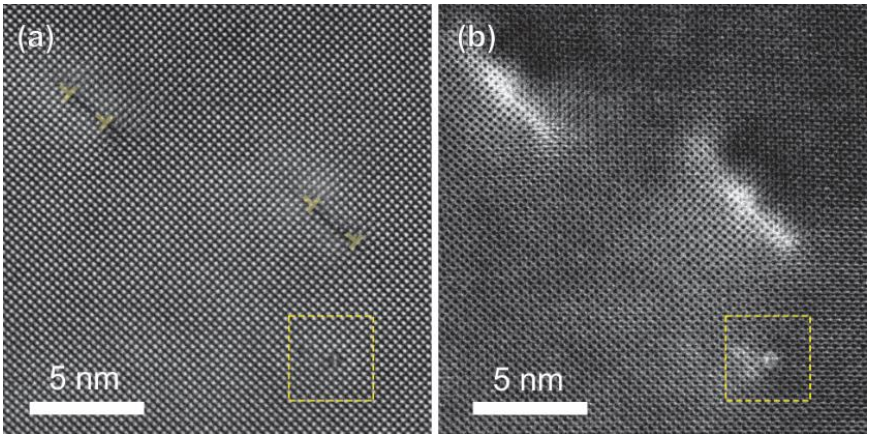

Figure 1. HAADF-STEM and LAADF-STEM images of the $BaSnO_3$ film in plan-view orientation. Typical edge dislocations are marked with the dislocation symbols in (a) and a unique line defect is highlighted in the yellow box in (a) and (b).

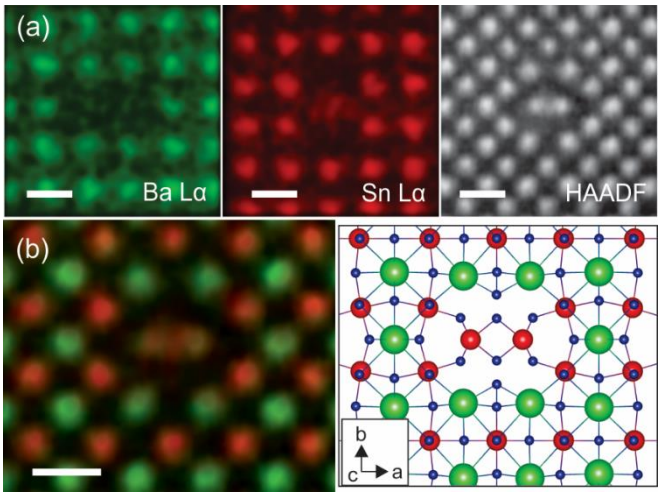

Figure 2. (a) EDX maps and HAADF-STEM image of the line defect. (b) The left panel shows the Ba (green) and Sn (red) maps overlaid on the HAADF-STEM image and the right panel shows a possible atomic configuration of the line defect. All scale bars are 0.4 nm.