doi:10.1017/S1431927618000831
Microsc. Microanal. 24 (Suppl 1), 2018
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Unique Line Defect Discovered in $BaSnO_3$ Thin Film

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Research of epitaxially grown thin films at the atomic scale has been performed in a daily routine, and defects with dimensions ranging from 0-D [1] to 3-D [2] have been widely explored. In particular, a recent discovery of a new line defect in $NdTiO_3$ hinted at the presence of more unique line defects in perovskite materials [3]. Here, we report a newly-discovered line defect in perovskite $BaSnO_3$ thin films. The line defect is formed along the film growth direction and shows a unique atomic configuration, compositionally and structurally different from the host $BaSnO_3$ perovskite crystal.

DC sputter deposition method was used to grow 200 nm-thick La-doped $BaSnO_3$ thin films on a $LaAlO_3$ substrate [4]. STEM experiments were carried out using FEI Titan G2 60-300 (S)TEM equipped with CEOS DCOR probe corrector, a Schottky extreme field emission gun (X-FEG), and a monochromator. The microscope was operated at 200 keV. The EDX spectra and elemental maps were acquired using the FEI Super-X EDX detector and EELS spectra were measured using the Gatan Enfinium ER spectrometer. Fig. 1(a) is a plan-view HAADF-STEM image from the $BaSnO_3$ film. The line defect is observed besides typical dislocations. LAADF-STEM image from the same region shows strong strain contrast around them (Fig. 1(b)). STEM-EDX elemental map acquired from one of the line defects is shown in Fig. 2. The elemental map reveals that two Ba columns are missing and two Sn columns fill the Ba positions. The chemical bonding and electronic structures of the core is different from a perfect crystal, so is its electronic structure. By utilizing EELS and DFT-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 [5], is discussed.

Along with the previously reported line defect in $NdTiO_3$, this study demonstrates that unique 1-D defects do exist in perovskite epitaxial films and raises more questions about mechanisms and conditions creating these peculiar defects, their effects on the material's overall electronic and magnetic properties, and their properties that possibly can be utilized by defect engineering [6].

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[6] We thank K. Ganguly, W. Postiglione, B. Jalan, and C. Leighton for $BaSnO_3$ films. This work was supported partially by the NSF MRSEC under Award Number DMR-1420013, Grant-in-Aid program of the University of Minnesota, and a fellowship from the Samsung Scholarship Foundation, Republic of Korea.

https://doi.org/10.1017/S1431927618000831 Published online by Cambridge University Press

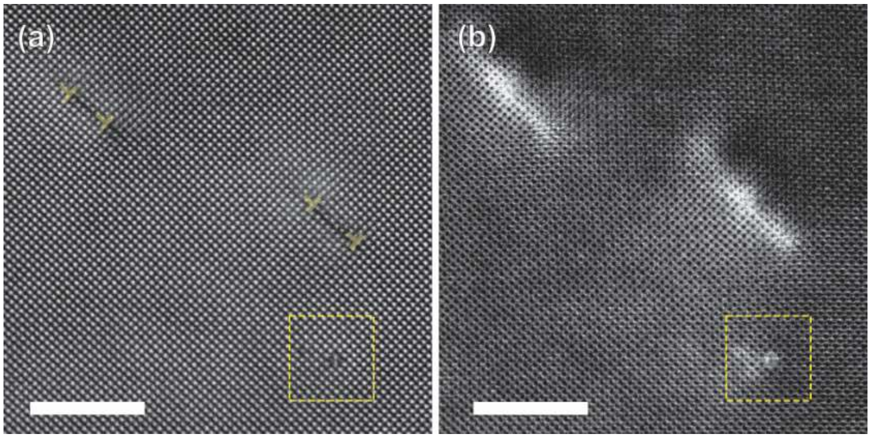

Figure 1. (a) HAADF-STEM and (b) LAADF-STEM images of the $BaSnO_3$ film in plan-view orientation. Typical threading dislocations are marked with dislocation symbols in (a) and a unique line defect is shown in the yellow box in (a) and (b). Scale bars are 5 nm.

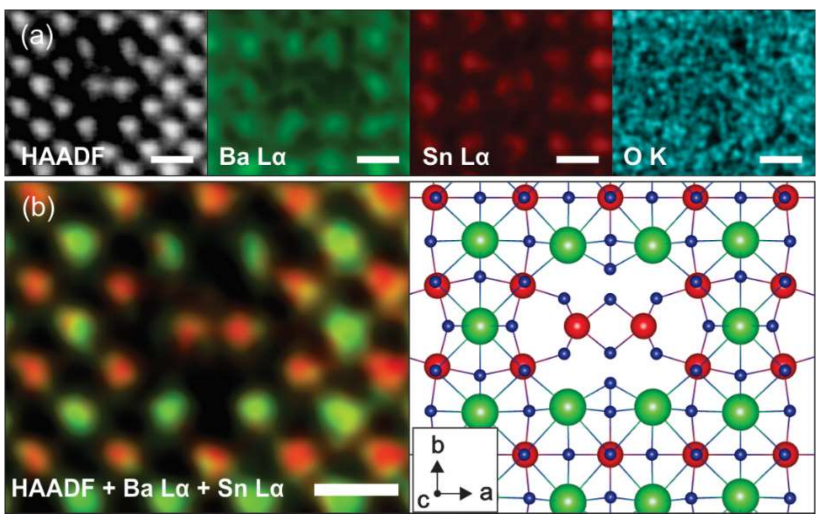

Figure 2. (a) HAADF-STEM image and elemental EDX maps of a line defect. (b) The left panel shows the Ba (green) and Sn (red) maps overlaid on the HAADF-STEM image and the right panel shows a possible atomic model of the line defect. All scale bars are 0.4 nm.

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