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Uncovering the Microstructure of $BaSnO_3$ Thin Films Deposited on Different Substrates Using TEM

Hwanhui Yun[1], Koustav Ganguly[1], William Postiglione[1], Bharat Jalan[1], Chris Leighton[1], K. Andre Mkhoyan[1] and Jong Seok Jeong[1]

[1]. Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN.

$BaSnO_3$ has been the subject of research since the discovery of its high carrier mobility at room temperature [1-3]. Particularly, $BaSnO_3$ epitaxial thin films have been widely studied, and the technology for their deposition has advanced rapidly [4]. The crystalline quality of thin $BaSnO_3$ films has been attributed as the main limiting factor for its electronic properties, especially, carrier mobility [4,5]. However, not much research has been done on in-depth microstructural characterization of $BaSnO_3$ thin films. In this study, the microstructures of $BaSnO_3$ films grown on two different perovskite substrates are investigated and compared using various TEM techniques.

La-doped $BaSnO_3$ films were grown on two substrates, $LaAlO_3$(001) and $PrScO_3$(001), by high pressure oxygen DC sputter deposition, targeting 200 nm-thick $Ba_{0.98}La_{0.02}SnO_3$ epitaxial layers [6,7]. CTEM images and electron diffraction patterns were acquired using FEI Tecnai G2 F30 (S)TEM at 300 keV, and ADF-STEM images were obtained using FEI Titan G2 60-300 (S)TEM at 200 keV. Plan-view and cross-sectional TEM samples were prepared by mechanical polishing and focused ion beam lift-out methods, respectively.

Rotational disorder, in-plane twists and out-of-plane tilts, were detected in the two films and visualized using two-beam conditions in CTEM mode, as shown in Fig. 1. The out-of-plane tilt of the grains was observed only in $BaSnO_3$ grown on $LaAlO_3$, and not in $BaSnO_3$ on $PrScO_3$, while the in-plane twist was observed in both films. Grains with the rotational disorder were identified, and their sizes were estimated from the images to be around 30 nm. The degree of rotational disorders was examined using electron diffraction patterns from cross-sectional and plan-view samples, and the results were compared with X-ray diffraction. The different microstructures between the two $BaSnO_3$ films on dissimilar substrates were explained by inspecting the atomic structures of the film-substrate interfaces (Fig. 2). $BaSnO_3$ on $LaAlO_3$, possessing larger lattice mismatch, showed a higher density of misfit dislocations at the interface than $BaSnO_3$ on $PrScO_3$. In addition, misfit dislocations with a Burgers vector along the film growth [001] direction were detected in $BaSnO_3$ on $LaAlO_3$, explaining the out-of-plane tilt observed. This study shows how to assess the rotational disorder in thin films and highlights the capabilities of various TEM techniques in studying the microstructures of such thin films [8].

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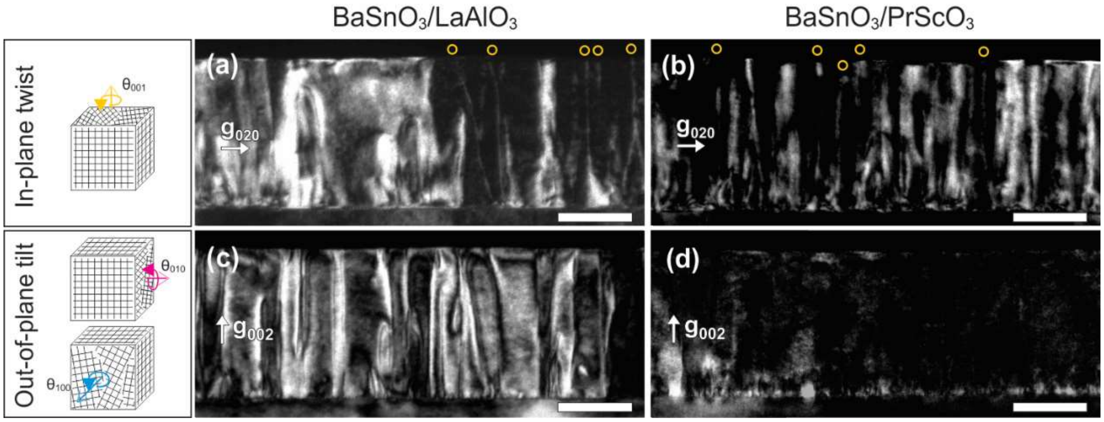

Figure 1. Cross-sectional two-beam dark field images of La-doped $BaSnO_3$ with (a,b) **g**=020 and (c,d) **g**=002. Schematics of corresponding rotational disorders are illustrated in the left column. All scale bars are 100 nm.

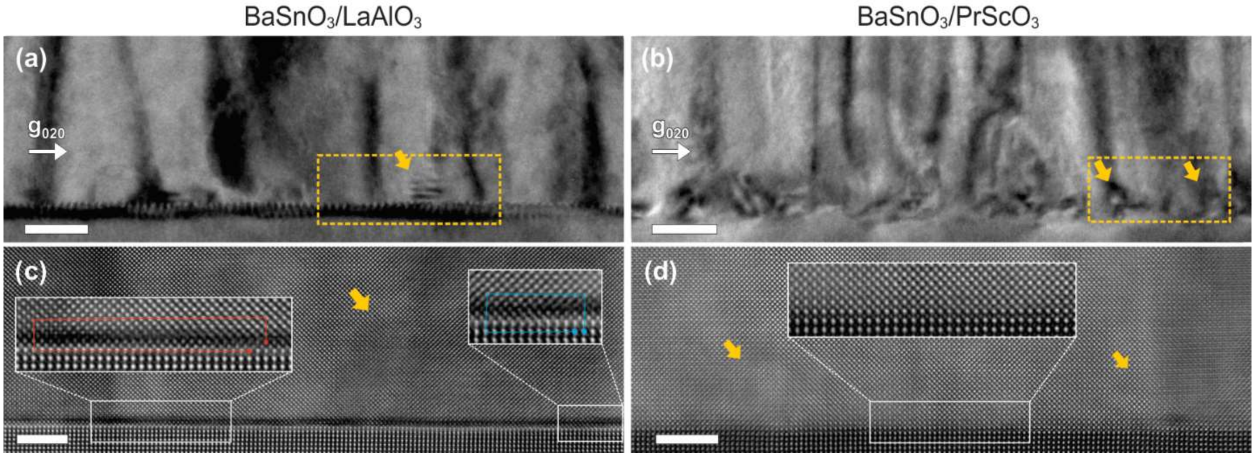

Figure 2. Cross-sectional TEM images of the $BaSnO_3$ films at the film-substrate interface. (a,b) Two-beam bright field images with **g**=020. Scale bars are 20 nm. (c,d) HAADF-STEM images obtained from regions inside the yellow dotted boxes in (a) and (b). Scale bars are 5 nm. Burgers circuits demonstrating misfit dislocations with **b**=[001] (red) and **b**=[010] (blue) are drawn in insets in (c). Misoriented small grains at the interface are marked with yellow arrows.