doi:10.1017/S1431927616002452
Microsc. Microanal. 22 (Suppl 3), 2016

Study of Strain and Intermixing at the $BaSnO_3/SrTiO_3$ and $BaSnO_3/LaAlO_3$ Interfaces Using STEM and EELS

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The interfaces between two different perovskite oxides have been widely studied since the discovery of metallic behavior at the interface of $SrTiO_3/LaAlO_3$ [1]. While various novel electronic properties, such as two-dimensional electron gas [2], superconductivity [3], and quantum hall effect [4], have been observed in some perovskite materials, the origins of these emergent properties are still under debate. More studies of these properties in perovskite materials are desired, and transparent and insulating cubic perovskite $BaSnO_3$ is a promising candidate for such studies. Recently, bulk $BaSnO_3$ reportedly showed unusually high carrier mobility at room temperature that was comparable to Si [5]. The heterostructures of $BaSnO_3$ with other perovskite oxides are also expected to exhibit unusual electronic properties. Motivated by this, we conducted scanning transmission electron microscopy (STEM) and electron energy-loss spectroscopy (EELS) studies of two $BaSnO_3$ interfaces: $BaSnO_3/LaAlO_3$ and $BaSnO_3/SrTiO_3$.

$BaSnO_3$ films were grown on a $SrTiO_3$ substrate by molecular beam epitaxy (MBE) [6] and on a $LaAlO_3$ substrate by high pressure oxygen sputter-deposition [7]. The film-substrate interfaces were analyzed using a FEI Tecnai G2 F30 (S)TEM equipped with Gatan Enfina-1000 electron energy-loss spectrometer, operated at 300 kV.

High-angle annular dark-field (HAADF) STEM investigation showed, in addition to the presence of expected epitaxial $BaSnO_3$ layers, regularly spaced strained regions, which originated from misfit dislocations. Figure 1 shows an example of one such HAADF-STEM image from $BaSnO_3/LaAlO_3$ sample. To further study possible emergent electronic properties across the interfaces, it is necessary to elucidate the effects of (1) the local lattice strain due to cation intermixing and (2) structural defects on the local electronic density of states. Core-level EELS Ba $M_{4,5}$-, La $M_{4,5}$-, and O K-edges, as well as low-loss EELS spectra, were recorded across the interface. Ba and La $M_{4,5}$-edges, consisting of two white line peaks (Figure 2), were analyzed to quantitatively evaluate the cation intermixing at the interface and to examine possible onset shifts. It was found that the cation intermixing occurs up to around 5 nm, which is farther than expected. O K-edge fine structure was also analyzed across the interface (Figure 3). Unlike bulk materials, a pre-peak was observed in the O K-edge in $LaAlO_3$ near the $BaSnO_3/LaAlO_3$ interface. A pre-peak in O K-edge has been known to result from hybridization between transition metal d orbital and O p orbital [8], which is sensitive to a local bonding between transition metals and O. Here, extensive STEM-EELS characterization at the interfaces using both the cation $M_{4,5}$-edges and O K-edge fine structures is conducted to study the strain and intermixing at the interfaces. The modification in the local electronic density of states resulting from strain at the interface is discussed after separating the intermixing effect [9].

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[9] This work was supported primarily through the NSF under Award No. DMR-1410888 and in part by NSF MRSEC under Award No. DMR-1420013. H.Y. acknowledges a fellowship from the Samsung Scholarship Foundation, Republic of Korea.

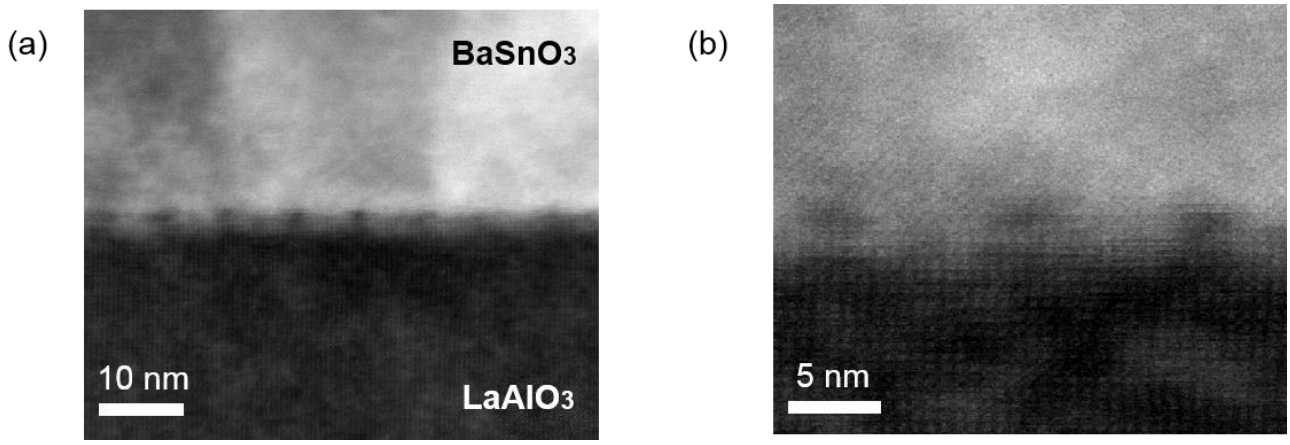

Figure 1. (a) HAADF-STEM image of strain field at the interface of $BaSnO_3$ and $LaAlO_3$. (b) High magnification image of the same region.

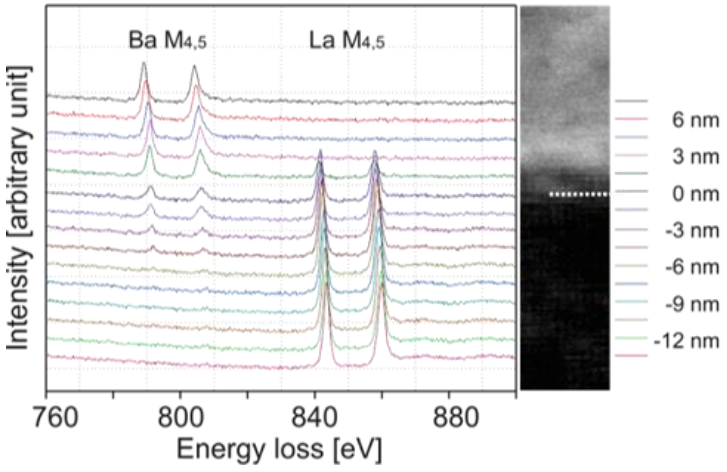

Figure 2. Ba and La $M_{4,5}$-edge EELS spectra obtained across the $BaSnO_3/LaAlO_3$ interface.

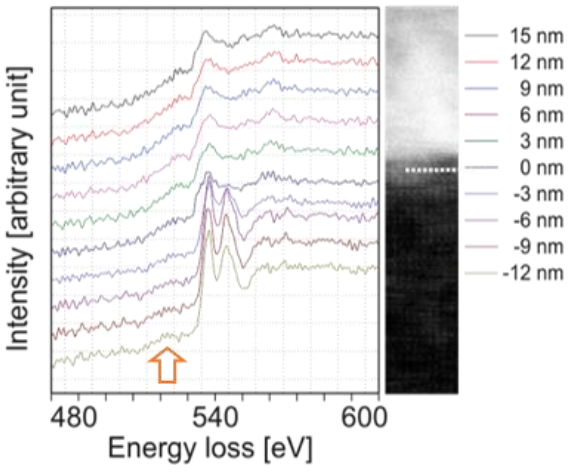

Figure 3. EELS fine structure of O K-edge. Pre-peaks were marked.

https://doi.org/10.1017/S1431927616002452 Published online by Cambridge University Press