

Electronic structure of BaSnO₃ investigated by electron energy-loss spectroscopy

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Electron energy-loss spectroscopy (EELS) is a powerful tool to explore the electronic structures of perovskite materials [1]. Low-loss EELS contains information about the band gap and dielectric response of the material, and core-loss EELS measures the core-electron excitations to the empty density of states above the Fermi energy [2]. When supplemented with first principle calculations, an extensive knowledge on the electronic structures of materials can be achieved. Here, the electronic structure of perovskite BaSnO₃, one of the promising materials for next generation oxide electronic devices [3], is explored using high-energy-resolution EELS and first principle calculations.

BaSnO₃ films used in this study were grown on SrTiO₃(001) substrates by a hybrid molecular beam epitaxy [4]. Subsequently, scanning transmission electron microscopy (STEM) imaging and EELS measurements were carried out using a monochromated and aberration-corrected FEI Titan G2 60-300 (S)TEM at 200 keV. The EELS spectra were acquired from cross-sectional STEM samples (Fig. 1) prepared using the focused ion beam lift-out method.

The valence band electronic structure of BaSnO₃ was investigated by a combination of low-loss EELS spectra and the dielectric function obtained from first principle calculations. Individual peaks in the experimental low-loss spectra showing plasmon excitations and interband transitions were matched to corresponding transitions as shown in Fig. 2(a). The bandgap of BaSnO₃ was also measured using the onset of the low-loss data.

Core-level electron excitations were explored through measurements of the core-loss EELS edges of O *K*, Ba *M*_{4,5}, Sn *M*_{4,5}, and Ba *M*_{4,5} edges. The simpler O *K* edge, resulting from the excitation of O 1*s* electrons to the empty density of states above the Fermi energy, was compared with a simulated O *K* edge generated using first principle calculations, where the cross-section of the O *K* edge modified by the core-hole effect is calculated with the natural energy broadening. The experimental O *K* edge EELS spectra are in excellent agreement with the simulated result, as shown in Fig. 2(b). This study demonstrates that EELS analysis can be a powerful tool for understanding the electronic structure of perovskite materials [5].

Reference

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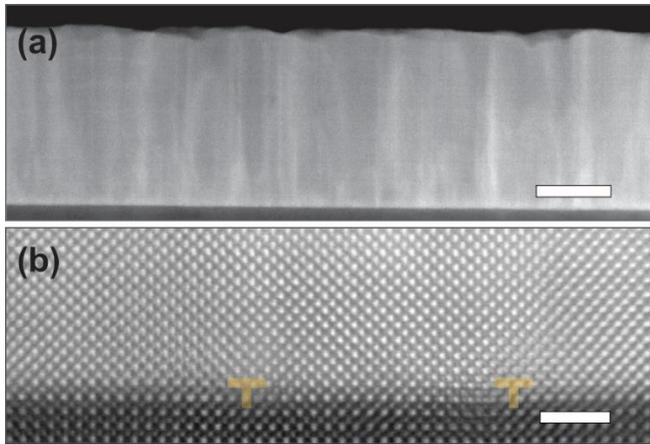


Figure 1. Cross-sectional high-angle annular dark-field (HAADF) STEM images of 200 nm-thick BaSnO₃ on LaAlO₃. Scale bars are 100 and 2 nm in (a) and (b), respectively. Misfit dislocations at the interface are marked with dislocation symbols in (b).

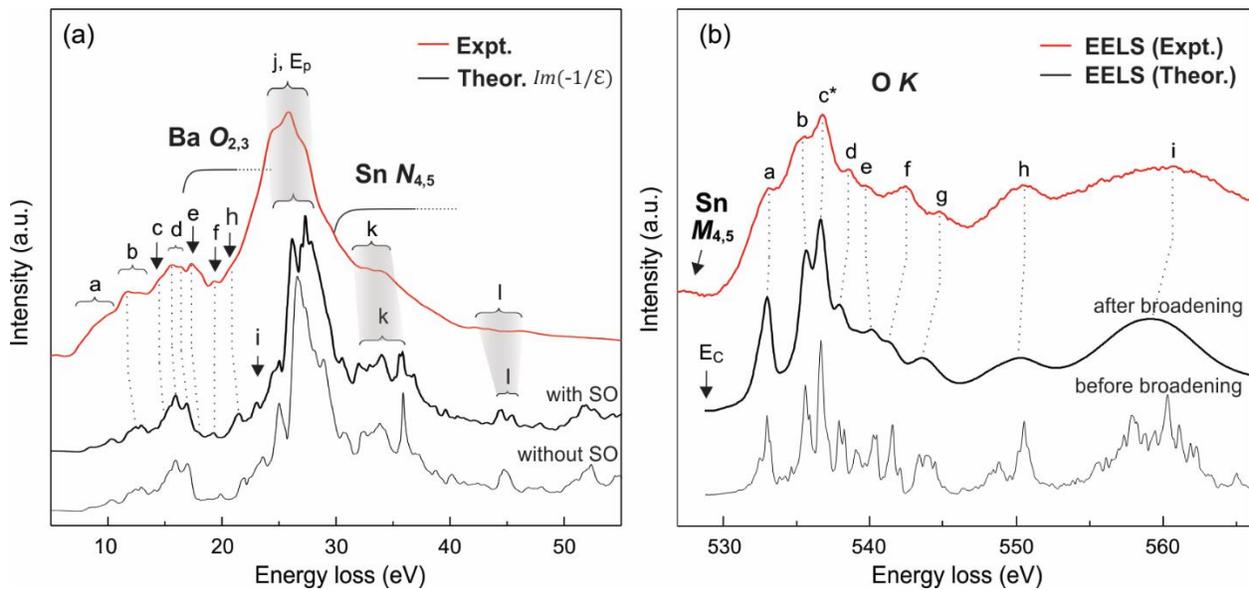


Figure 2. Experimental (red) and theoretical (black) EELS spectra of BaSnO₃. (a) Low-loss EELS spectra. Identifiable peaks are labeled from a to l and plasmon peak is indicated by E_p . Core-edges in the low-loss region - Ba O_{2,3} and Sn N_{4,5} - are indicated. (b) O K EELS spectra. Major peaks are labeled from a to i. Theoretical EELS spectra, before and after natural energy broadening, are displayed. E_c is the onset of the O K edge.