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Probing the Electronic Structure of $BaSnO_3$ by EELS Analysis and *ab initio* Calculations

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Revealing the electronic structure of materials is essential in understanding their properties. While there are many experimental methods [1-3] for evaluating key parameters of electronic and optical properties of materials, we note that electron energy-loss spectroscopy (EELS) can provide comprehensive information on the electronic structure of materials [4]. In this study, the electronic structure of perovskite structure $BaSnO_3$, one of the promising materials for next generation oxide electronic devices, is explored using high-energy-resolution EELS and *ab initio* calculations.

$BaSnO_3$ films were grown on $SrTiO_3$(001) substrates by molecular beam epitaxy (MBE) [5] and on $LaAlO_3$(001) substrates by high pressure oxygen sputter-deposition (Figure 1) [6]. 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, equipped with a CEOS DCOR probe corrector, a Schottky extreme field emission gun (X-FEG), a monochromator, and a Gatan Enfinium ER spectrometer. The microscope was operated at 200 keV [7].

The bandgap of $BaSnO_3$ was measured from the onset of low-loss EELS data. The valence band electronic structure was investigated by a combination of low-loss EELS spectra and the dielectric function obtained from *ab initio* calculations. Low-loss EELS spectra were compared with the electron energy loss function, which is the imaginary part of the inverse dielectric function (Figure 2). Peaks from Plasmon excitations and interband transitions were observed, and interband transition peaks were further resolved by inspecting the band structures calculated by the *ab initio* method and assigning corresponding interband transitions to observed peaks. The core-level electron excitations were also explored using the core-loss EELS edges of O *K*, Ba $N_{4,5}$ Sn $N_{4,5}$, and Ba $M_{4,5}$ edges. A 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 the O *K* edge simulation result generated using the *ab initio* calculations. The experimental O *K* edge EELS spectra are in very good agreement with the simulation result, as shown in Figure 3. Our study demonstrates that EELS analysis can be a powerful tool for understanding the electronic structure and properties of materials [8].

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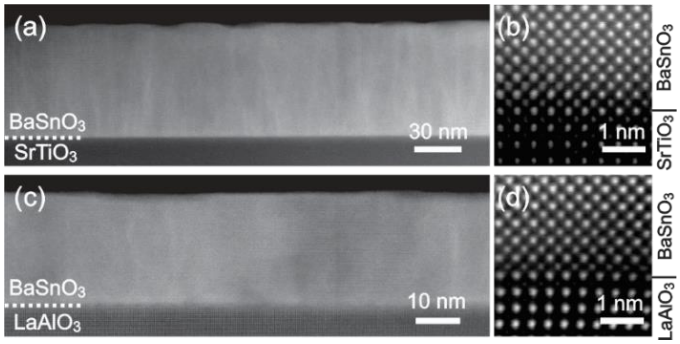

Figure 1. Low-magnification and high-resolution HAADF-STEM images of $BaSnO_3$ films: (a,b) $BaSnO_3$ film grown on a $SrTiO_3$ (001) substrate and (c,d) $BaSnO_3$ film grown on a $LaAlO_3$ (001) substrate.

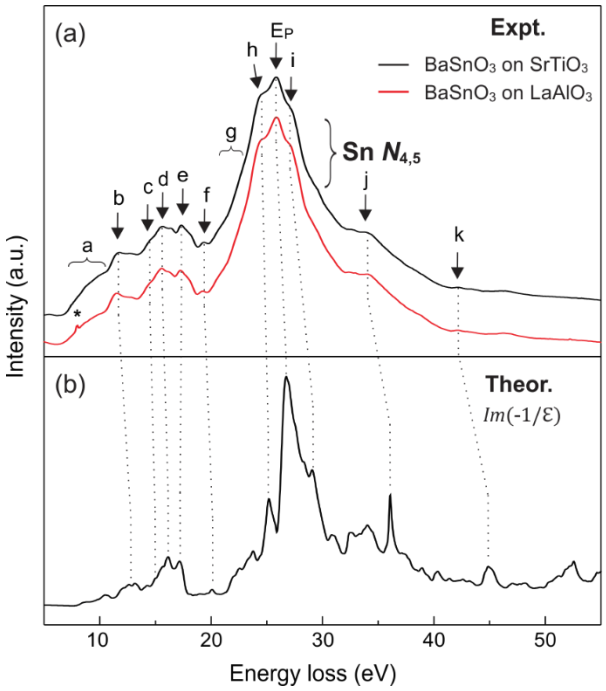

Figure 2. Comparison of experimental low-loss EELS spectra from the two $BaSnO_3$ films (a), and calculated Im[-1/ε] (b). The peaks from interband electronic transitions are labeled from a to k. The bulk plasmon peak, Ep, and the Sn $N_{4,5}$ edge are also indicated.

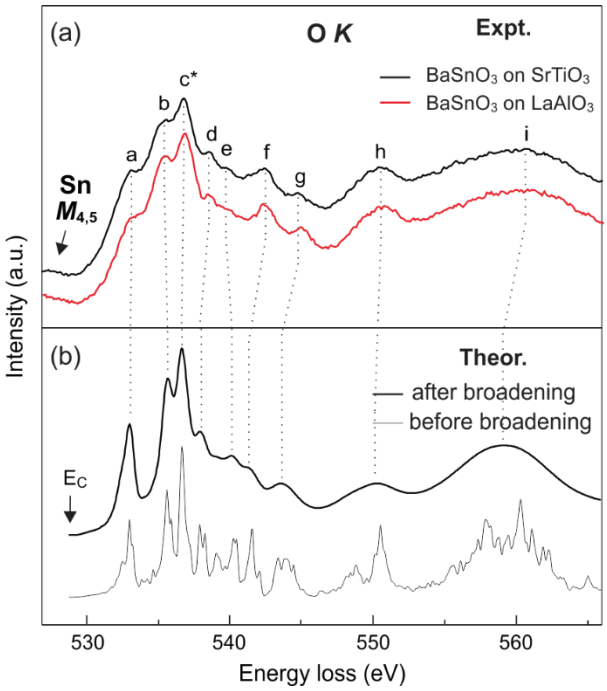

Figure 3. Comparison of experimental EELS O *K* edges from two $BaSnO_3$ films (a) and simulated O *K* edge (b): (a) The peak c* was used as a reference for the alignment.(b) Before (thin line) and after (thick line) implementing beam and energy broadening.

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