Trends in the O K edge for perovskite oxides: a tool for extracting interfacial properties

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Perovskite oxides have attracted significant attention due to a wide range of potential device applications. Electron Energy Loss Spectroscopy (EELS) in a Scanning Transmission Electron Microscope (STEM) has proven to be a powerful tool for the characterization of oxide interfaces, grain boundaries and dislocation cores which play an important role in determining the bulk properties of these materials. However, a good understanding of the near edge fine structure of the energy loss spectra is essential. In this context, we have been studying the trends in the O K edge for various perovskite oxides. We find that the first peak in the O K edge is mainly determined by the valence state of the transition metal, whereas the second peak in the O K edge is attributed to states derived from oxygen p and the A-site cation d orbitals.

Fig. 1b is an annular dark field STEM image of a low-angle twist grain boundary between SrTiO3 and Nb:SrTiO3. The tilt of ~2° between the two crystals induces the formation of screw dislocations at the interface with an average spacing of 113Å. The observed dislocations adopt a more open core structure than recently reported for screw dislocation in SrTiO3 [1] possibly due to different annealing conditions. The chemistry of the dislocation core was measured on the atomic scale using Ti L2,3 (Fig. 1a) and O K edge (Fig. 1c) EELS in a STEM. The Ti L2,3 edge on the dislocation core reveals a reduction of the formal Ti oxidation state from 4+ in bulk SrTiO3. Fig. 1c shows O K edge spectra on and off the dislocation core. We observe a strong reduction of the second peak, suggesting Sr deficiency of the dislocation core.

FIG. 1. Screw dislocations at the STO/Nb:STO interface: (a) Ti L2,3 edge spectra, (b) ADF-STEM image and (c) O K edge spectra with energy resolution of 0.8eV.

References
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