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Low energy-loss spectroscopic studies of grain boundary cores in complex oxides.

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In the nanoscience era, the characterization of the structure and electronic properties of matter at the atomic scale is becoming ever more vital for economic and technological as well as scientific reasons. The combination of atomic-resolution Z-contrast scanning transmission electron microscopy (STEM) and electron energy loss spectroscopy (EELS) represents a powerful method to link the atomic and electronic structure to macroscopic properties, allowing materials, nanoscale systems and interfaces to be probed in unprecedented detail. Recent developments in aberration correction have pushed the achievable spatial resolution and the sensitivity for imaging and spectroscopy in STEM into the sub-Angstrom regime, providing a new level of insight into the structure/property relations of complex materials. Interestingly, very few experimental studies have been reported to address the structure/property relationships of materials by means of analyzing the low-loss region of the electron energy loss spectra (EELS). While the electronic excitations in this regime are more spatially delocalized than the higher energy core loss excitations, the higher intensity and therefore, shorter acquisition times make the low-loss EELS useful when it comes to quantifying the chemistry/electronic properties of nanomaterials, defects and interfaces with sub-nanometer resolution.

In this work, we address the quantification of the electronic structure [1], optical properties [2] and chemical composition across dislocation cores of a low angle grain boundary (GB) in $SrTiO_3$ (STO) by using low-loss spectroscopy. Short acquisition times allow the acquisition of relatively large spectrum images which make possible to create elemental mappings similar to those obtained by energy filtered transmission electron microscopy. As an example, Figure 1 shows a Z-contrast image of a 12° grain boundary in STO. The dislocation cores can clearly be seen. Figure 2 shows the low-loss energy-loss spectra obtained from the bulk and when placing the electron beam on the GB core. Results on the mapping of chemical composition of the dislocation cores will be presented, which is a key issue, as previous studies showed that these dislocation cores are non stoichiometric [3]. The local electronic and properties are obtained from the low loss spectra, such as the band gap widths, index of refraction, etc. It will be shown how these and other properties can be mapped quantitatively as a function of position relative to the grain boundary cores.

References

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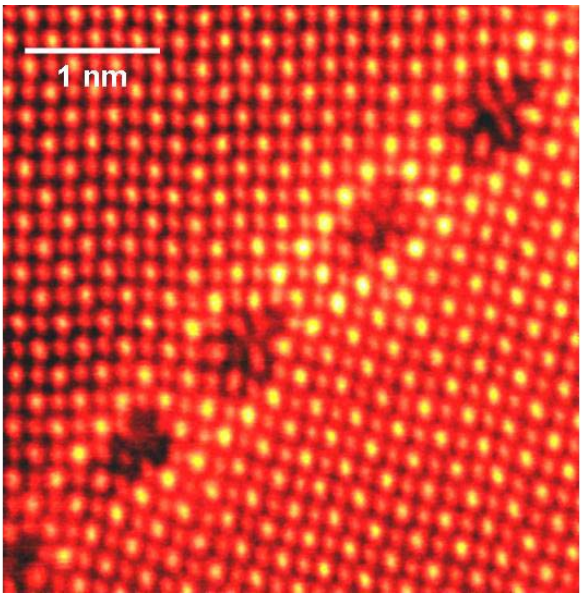

FIG. 1. Z-contrast image of a 12 degree grain boundary in SrTiO3, showing the arrangement of dislocation cores.

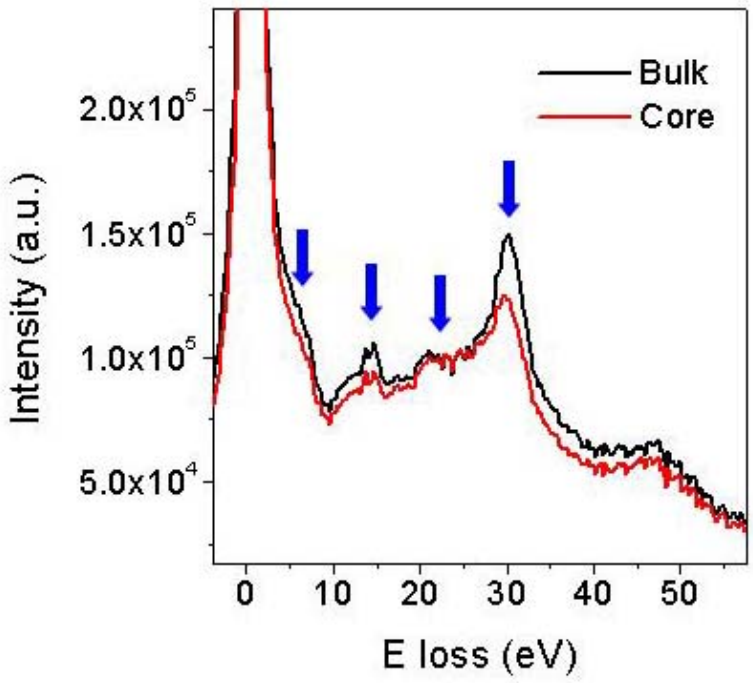

FIG. 2. Low energy-loss spectra from the bulk (black) and from the dislocation core (red). Blue arrows mark areas where the main differences observed.

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