

Surface band gap narrowing in ferroelastic domain walls

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We have measured the band gap in domains and at domain walls on the surface of ferroelastic CaTiO₃ (001) using Electron Energy Loss Spectroscopy (EELS). We observe that on the surface, the band gap is smaller in the domain walls than in adjacent domains.

CaTiO₃ is a perovskite oxide with an orthorhombic lattice. As a pure ferroelastic material, the order parameter is the strain defined by the oxygen octahedral tilts in the unit cell. At the domain walls, octahedral tilt goes to zero, allowing the central Ti cation to off-center, creating polarity.

We first confirmed domain wall polarity from MEM-LEEM transition maps. Then, the band gaps are extracted from the EELS spectrums as shown spectra, taken in of the domains and domain walls are extracted using from areas defined by a field aperture. The band gap is the energy separation between the elastic peak position and the onset of the secondary electron peak. The measured band gap for For the domain walls 1, 2 and 3 are it is 3.82, 4.11, 4.28 eV, respectively. In every case, it is smaller in the domain wall than in the adjacent domains. The results confirms that the emergence of polarity in the domain walls is correlated with a change in the local electronic structure. The narrowing may be due to the different symmetry existing in the domain walls [1] and/or the presence of oxygen vacancies, which are diffusing and concentrate in the domain walls [2]. This may be of importance in the perspective of using the twin wall functionality for microelectronics applications.

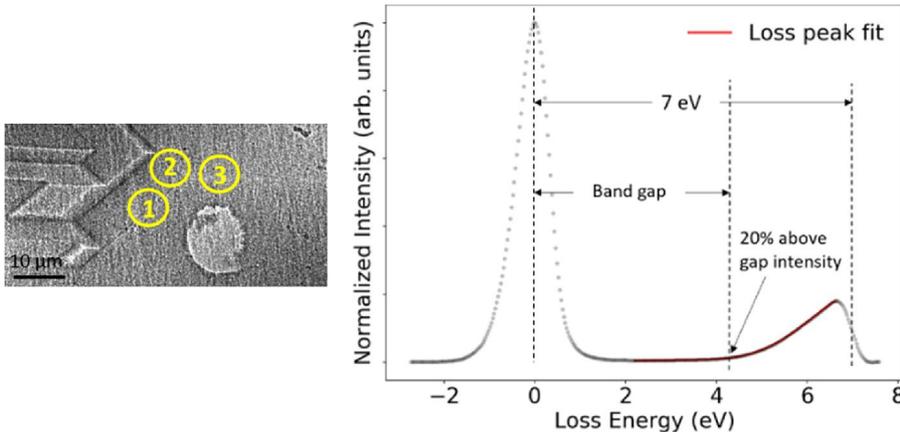


Figure 1. (left) Image of the surface of CaTiO₃ with the position of the EELS measurements. Dark domain walls are upward pointing and white walls are downward pointing polarity [3]. The yellow circles indicate the field aperture positions used to define the area of the EELS spectra (right) EELS spectra from domain wall 1 with an incident energy of 7 eV.

References

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