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Atomic-scale imaging of flexoelectric polarization around engineered crack tips

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As a universal electromechanical coupling effect, the flexoelectric effect describes the response of electric polarization to a mechanical strain gradient. Unlike the piezoelectric effect, which only emerges in non-centrosymmetric materials, flexoelectricity even appears in centrosymmetric materials. The study of flexoelectricity has been reported in various materials, including common solids, liquid crystals, and biological materials [1]. Nevertheless, the flexoelectric effect is very weak in bulk materials, because strain gradients are typically small [2]. In nanoscale structures, however, larger strain gradients are possible, and flexoelectric polarizations comparable to those of ferroelectric materials can be achieved, playing an important role in modifying the functional properties of materials [3]. Benefited from the advances in material fabrication and characterization, nanoscale flexoelectricity has been a research hotspot in recent years.

In our work [4], SrMnO3 (SMO) epitaxial thin films were grown on TiO2-terminated (001)-oriented SrTiO3 (STO) substrates by pulsed laser deposition. SMO grows very well on STO, resulting in a coherent epitaxy at the growth temperature, i.e. 800 °C. However, when we reinvestigated the samples at a later stage, cracks appeared to relax the thermal strain [5]. The time scale for the crack formation depends on the thicknesses of the thin films. An SEM image in the upper-right panel of Figure 1 clearly shows straight cracks aligned with the [100] and [010] crystal-lattice directions. The averaged separation of the cracks in the SEM image is ∼100 nm, and the cracks are continuous for lengths of 100−2000 nm.

Aberration-corrected scanning transmission electron microscopy (STEM) and spectroscopy were then carried out to unravel the atomic structure, strain distributions, and electronic structure around crack tips. Based on quantitative STEM analysis, we mapped the strain field around the tip of deep cracks penetrating into STO substrates crack tips (Figure 2). It shows a large strain gradient with a magnitude as high as 3.0 nm−1. We then realize a direct mapping of the electrical polarization within three unit cells around the crack tip (bottom-left panel in Figure 1) through a precise determination of atomic-column positions by fitting Gaussian functions. The electrical polarization increases upon approaching the crack tip. The tip of the crack acts as a 180° domain wall with a head-to-head configuration, and the averaged polarization around the crack tip is as high as 62 ± 16 μC cm−2. Since the sign and size of the observed polarization match well with that of the strain gradient, we attribute the polarization to the flexoelectric effect. Moreover, we observe a valence state change of −0.7 ± 0.1 of the Ti ions at the tip of the crack, screening the flexoelectric polarization field.

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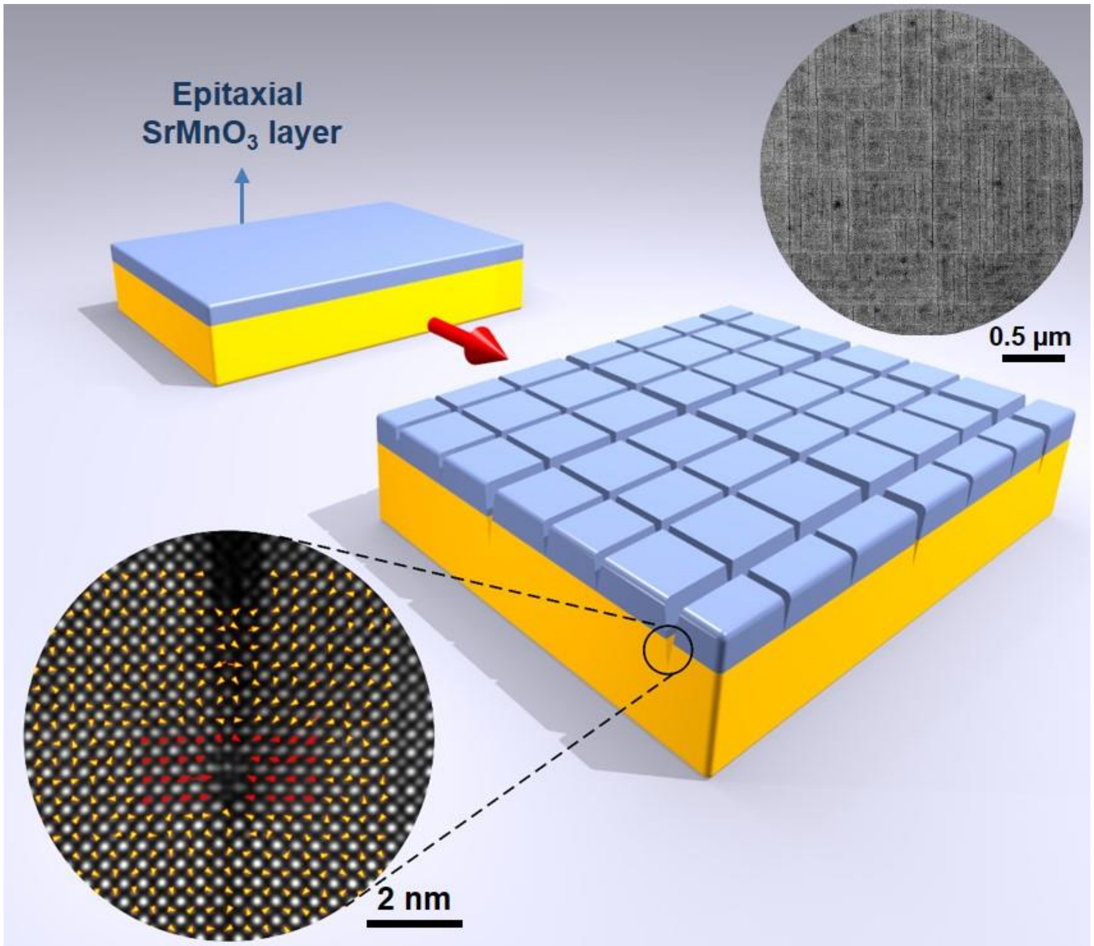

Figure 1. Schematic illustration for the flexoelectricity around engineered crack tips. As evidenced by the SEM image of the film's surface in the upper-right panel, straight cracks aligned with the [100] and [010] crystal lattice directions occur due to thermal-strain relaxation. Flexoelectric polarization around crack tips is visualized by the atomically resolved STEM image in the bottom-left panel.

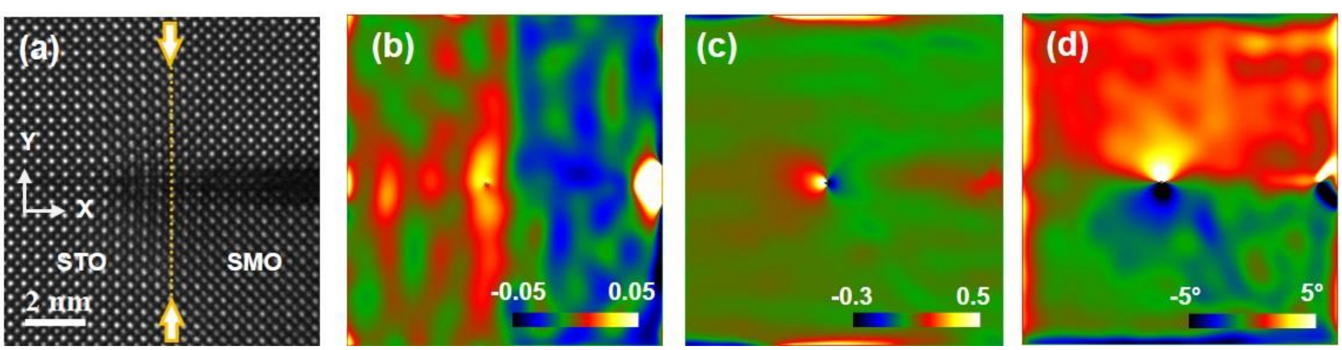

Figure 2. Geometric phase analysis of deep crack penetrating into SrTiO3. (a) The HAADF-STEM image of the deep crack. (b), (c), (d) are the in-plane strain map (εyy), out-of-plane strain map (εxx) and lattice rotation map (Rxy) around the crack tip.

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