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Functional domain walls in ferroelectric Pb(Zr1-xTix)O3 single crystals and thin films

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In recent years, ferroelectric domain walls (DWs) have been found to possess exceptional physical properties that are distinct from those of domains and enable them to play a role as functional entities in nanoelectronic devices[1]. This technological potential motivates the intense exploration of the internal structure of the DWs (on a unit-cell scale) and the DW response to external fields [2,3]. Investigated by (scanning) transmission electron microscopy ((S)TEM), the structure and behavior of DWs in two material systems of Ti-rich Pb(Zr1-xTix)O3 (PZT) single crystals and thin films are presented in this talk.
(1) By using negative spherical-aberration imaging (NCSI) technique, our atom-resolved TEM study reveals Néel-like DWs in Ti-rich (x = 0.54, 0.60) PZT single crystals (see Fig. 1(a,b)), in which nanometer-scale monoclinic order coexists with tetragonal order. Our quantitative TEM study, combined with phase-field simulation, concludes that charging and clamping effects at phase boundaries promote formation of the Néel-like DWs[4]. Discovery of the continuous polarization rotation not only provides a foundation for exploring chiral DWs in ferroelectrics, but also facilitates the development of miniature piezoelectric devices based on such DWs.
(2) In x = 0.9 PZT thin films, our annular-bright-field (ABF) STEM study reveals that charging of the ferroelastic 90° DWs can be controlled by mutually coupled DW bending, type of doping, polarization orientation and work-function of the adjacent electrodes (see Fig. 1(c,d)). In particular, the doping dominates over other parameters in controlling the DW conductivity[5]. Understanding the interplay between these parameters in the PZT films allows us to control and optimize conductivity of such ferroelastic DWs in the oxide ferroelectrics. Furthermore, it also paves the way for utilization of DWs in future nanoelectronic devices.

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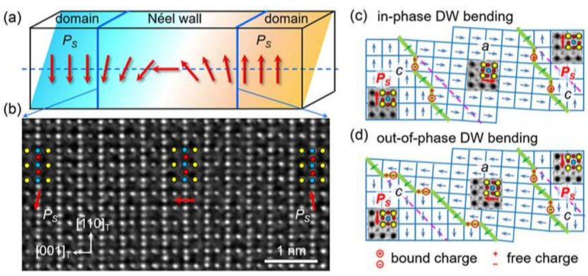

Figure 1. (a) Schematic representation of a Néel-type DW. (b) The Néel-like DW imaged in x = 0.60 PZT crystal. (c) The in-phase and (d) out-of-phase bent ferroelastic DWs in the x = 0.9 PZT thin films.