

Imaging pressure-nucleated and field-erased BiFeO₃ domains via in-situ nano-XRD

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Domains and their walls are functional units that play a central role in energy storage and electromechanical switching. Imaging these nanoscale units and tracking their dynamic response remains a major experimental challenge. Specifically, domains in thin-film device geometries are typically smaller than 100 nm and buried beneath metallic electrodes, making them inaccessible to conventional surface probes.

Nano-focused XRD offers sub-100 nm spatial resolution imaging of buried domains with both lattice strain and tilt sensitivity. We have recently exploited this capability to image ferroelastic-ferroelectric domains in BiFeO₃-based thin films in a capacitor geometry, uncovering how the mere electrode deposition introduces internal stress and domain reorientation [1]. The long penetration depth of the hard X-rays makes this method ideal for in-situ and operando experiments.

Here, we use in situ nano-indentation to locally transform the crystal structure of La-substituted BiFeO₃ from pseudocubic to orthorhombic, corresponding to a dipolar transition from ferroelectric-to-antiferroelectric state through stress-driven redistribution of La cations [2,3]. Furthermore, we use in-situ electric field applications to erase the transformed regions, tracking the evolution at the single-domain level.

Using scanning nano-XRD at the NanoMAX beamline, we map the evolution of strain and tilt heterogeneities across both stimuli, capturing in real space the nucleation and annihilation of ferroic order under competing mechanical and electrical drives. We discuss our recent finding on how the strain field impact the microscopic mechanisms of the phase transition and its reversal, offering new insight into the interplay between stress, lattice distortion, and polarization in oxide thin films for electronic applications.

References

- [1] Hill Landberg, M.O.; Yan, B.; Chen, H.; et al. Direct Imaging of Nanoscale Ferroelectric Domains and Polarization Reversal in Ferroelectric Capacitors. *Nano Lett.* 25, 16304–16310, 2025.
- [2] Mundy, J.A.; Grosso, B.F.; Heikes, C.A.; et al. Liberating a Hidden Antiferroelectric Phase with Interfacial Electrostatic Engineering. *Sci. Adv.* 8, eabg5860, 2022.
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