

The Growth of Super-Tetragonal Phase in BiFeO₃ on LaAlO₃ Substrate through Designer Defects

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Bismuth ferrite (BiFeO₃ - BFO) is one of the few known room temperature multiferroics¹ and it offers fascinating possibilities in applications ranging from spintronics,^{2,3} ferroelectric memories,⁴ light harvesting,⁵ optics,⁶ to hybrid devices.

A peculiarity of BFO is that its epitaxial growth under strong (>4%) compressive strain leads to the stabilization of a metastable multiferroic tetragonal T' phase.⁷ However, increasing the thickness of the BFO layer to greater than ~30 nm induces a strain relaxation mechanism, whereby a complex phase mixture of the metastable T' and a more stable R' like phase is formed.⁷ So far, the phase-field control of the various isomorphs of BFO and the tuning of their proportions has been achieved through modification of physical parameters, such as via substrate alternation and/or growth thickness. Control of phases using chemical phenomena has been vastly unexplored.

In this project, we have successfully grown BFO thin film on LaAlO₃ (001) (LAO) substrate with stabilized super-tetragonal phase for thickness > 70nm under ultra-low incident flux conditions in pulsed laser ablation growth. The presence of the T phase is confirmed through high resolution x-ray diffraction (XRD) and Cs corrected scanning transmission electron microscope (STEM). It is suggested that under these ultra-low incident flux conditions, the BFO thin film favor the formation of nanoscale 'defect pockets'. These 'defect pockets' can act as buffer layers to maintain macroscale strain coherence mechanical boundary conditions and stabilizes the T'phase, as they impose a net compressive strain of ~1.8% on BFO. By intentionally inducing defects, both in the stoichiometry and structure, we specifically enable the synthesis of BFO isomorphs in thickness regimes where normally strain relaxation would be expected to create BFO mixed phases. Finally, by intentionally introducing an amorphous phase at the film-substrate interface, we have shown that the mixed-phase proportion can be tuned for a given thickness.

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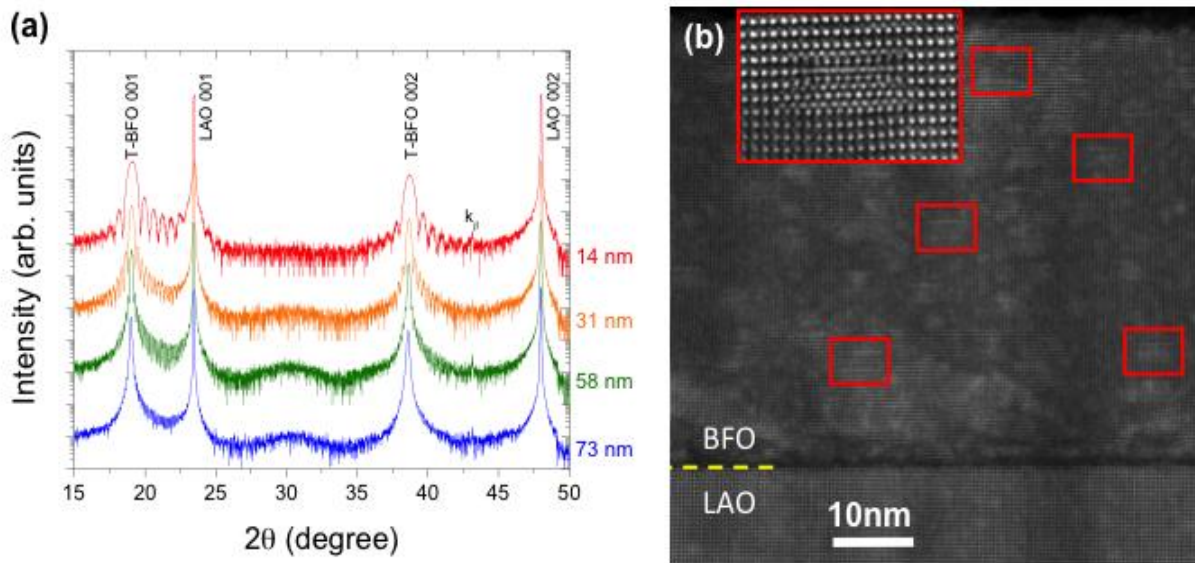


Figure 1 (a) X-ray diffraction coupled θ - 2θ scans of T' BiFeO₃ thin films grown by PLD. The broad structure at $2\theta \sim 30^\circ$ indicates the presents of defect pockets. (b) The scanning transmission electron microscopy (STEM)-high angle annular dark field (HAADF) image shows the presence of nano-pockets throughout the film (the inset shows an enlarged view of one such region).