Short range biaxial strain relief mechanism within epitaxially grown $BiFeO_3$

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$BiFeO_3$ (BFO) epitaxial films change crystal symmetry on the various single crystal substrates.[1)] Although the growth mechanism depends on each substrate, there is not so many detail and systematic structural analysis using various angle of electron diffraction combined with X-ray diffraction. In this study, lattice mismatch-induced biaxial strain effect on the crystal structure and growth mechanism is investigated for the BFO films grown on $La_{0.6}Sr_{0.4}MnO_3/SrTiO_3$ and $YAlO_3$ substrates. Nano-beam electron diffraction (NBED), structure factor calculation confirms that the crystal structure within both of the BFO thin films is rhombohedral by showing the rhombohedral signature Bragg's reflections. X-ray reciprocal space mapping (XRSM) unambiguously consistent with NBED. **[Fig. 1]** Further investigation with atomic resolution scanning transmission electron microscopy (STEM) reveals that while the ~1.0% of the lattice mismatch found in the BFO grown on $La_{0.6}Sr_{0.4}MnO_3/SrTiO_3$ is exerted as biaxial in-plane compressive strain with atomistically coherent interface, **[Fig. 1]** the ~6.8% of the lattice mismatch found in the BFO grown on $YAlO_3$ is relaxed at the interface by introducing dislocations. The present result demonstrates the importance of: (1) identification of the epitaxial relationship between BFO and its substrate material to quantitatively evaluate the amount of the lattice strain within BFO film and (2) the atomistically coherent BFO/substrate interface for the lattice mismatch to exert the lattice strain. [2)]

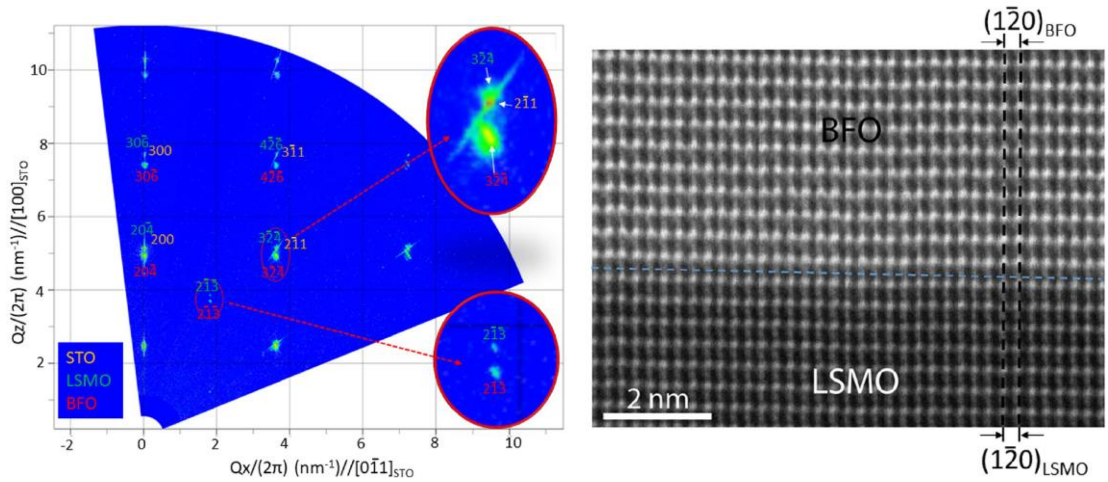

Fig. 1 A XRSM data of the BFO film grown on LSMO/STO substrate, and A cross-sectional HAADF-STEM image at the BFO/LSMO interface along [011] STO zone axis

[Ref]1) I.-T. Bae *et al.*, Jpn. J. Appl. Phys., **57**, 0902A5 (2018). 2) I.-T. Bae *et al.*, Sce. Rep. **9**, 6715 (2019).
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