Lattice mismatch effect on biaxial strain exerted on epitaxially-grown $BiFeO_3$

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Lattice mismatch-induced biaxial strain effect on the crystal structure and growth mechanism have been investigated. [Fig. 1] [1-3] for the $BiFeO_3$ thin 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 and X-ray reciprocal space mapping (XRSM) unambiguously confirm that the crystal structure within both of the $BiFeO_3$ thin films is rhombohedral by showing the rhombohedral signature Bragg's reflections. Further investigation with atomic resolution scanning transmission electron microscopy reveals that while the ~1.0% of the lattice mismatch found in the $BiFeO_3$ grown on $La_{0.6}Sr_{0.4}MnO_3/SrTiO_3$ is exerted as biaxial in-plane compressive strain with atomistically coherent interface, the ~6.8% of the lattice mismatch found in the $BiFeO_3$ grown on $YAlO_3$ turns out to be relaxed at the interface by introducing dislocations. The present result demonstrates the importance of: (1) identifying the epitaxial relationship between BFO and its substrate material to quantitatively evaluate the amount of the lattice strain within BFO and (2) the atomistically coherent BFO/substrate interface for the lattice mismatch to exert the lattice strain.

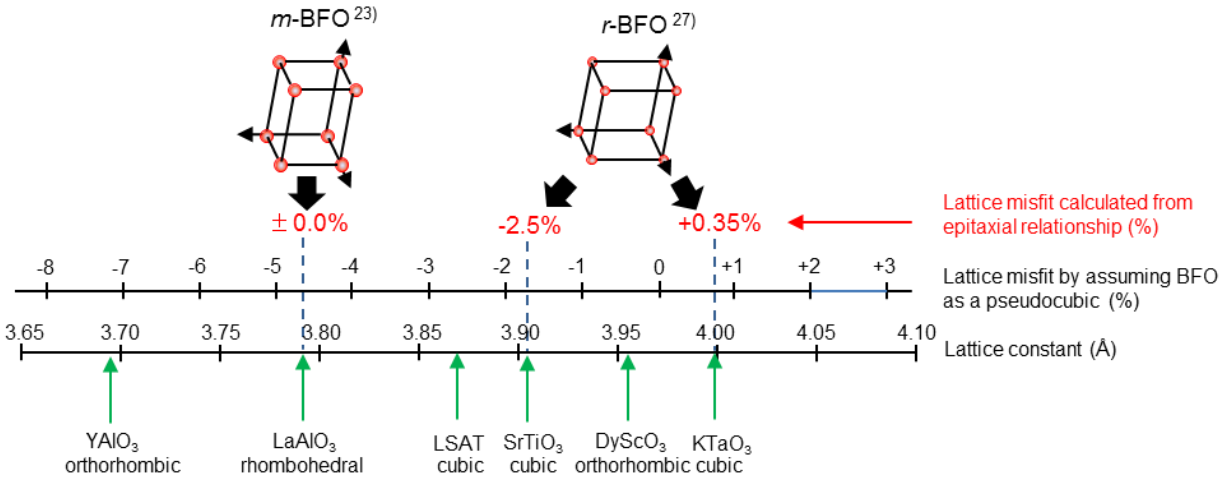

Figure 1 BFO lattice misfit values calculated based on epitaxial relationship with LAO, STO, and KTO substrates (in red). BFO lattice misfit values by assuming BFO as a pseudocubic are shown as well (in black) for comparison. (I. -T. Bae *et al.*, JJAP STAP review, 57, 0902A5 2018)

References) [1] I.-T. Bae and H. Naganuma, Appl. Phys. Express **8** (2015) 031501. [2] I.-T. Bae, et al., Sci. Rep. **7** (2017) 46498. [3] I.-T. Bae, T. Ichinose, M.-G. Han, Y. Zhu, S. Yasui, and H. Naganuma, Sci. Rep. **8** (2018) 893.