Biaxial tensile stress effect within epitaxial $BiFeO_3$ film grown on (100) $KTaO_3$

Bae, I.[1]

[1] State University of New York at Binghamton, United States

$BiFeO_3$ (BFO) is a multiferroic material with ferroielctricity and antiferromagnetsm showing up above room temperature. When BFO is grown thin film, its physical properties are known to dramatically change through biaxial stain applied from substrate materials. Since biaxial strain effects on crystal as well as microstructures within BFO film are closely related to physical property changes, extensive efforts have been devoted to investigate the effect of biaxial strain on crystal structural changes in BFO thin film. As a result, BFO film is reported to epitaxially grow as various phases such as rhombohedral, tetragonal-like, orthorhombic, monoclinic, and triclinic. However, because of remarkable structural complexity, the details about crystal structures in BFO films still remain an open question. It is worth noting that most of the previous experimental studies have utilized x-ray diffraction (XRD) based techniques making discussions about lattice distortion and/or lattice size changes. While XRD technique is excellent in providing volume-averaged lattice stress or strain with exceptional precision, the technique does not readily deliver wide range reciprocal lattice space information, which is critically important to evaluate overall crystal structure in thin film crystals. On the other hand, transmission electron microscopy (TEM) technique readily provides two-dimensional reciprocal information as wide as Q (scattering vector) = ~220 nm^{-1}. Furthermore, if TEM technique is combined with structure factor calculation, it has advantage over x-ray scattering technique in that not only lattice distortion and/or lattice size change, but also *locations of each basis atom* in unit cell can be precisely determined. This is particularly important for complex oxide materials such as BFO because slight location change in each constituent atom can cause extra Bragg's reflections at unexpected locations in reciprocal space.

The objectives of this work are as follows: (1) to investigate biaxial tensile stress effect on the crystal structure within epitaxial BFO film grown on $KTaO_3$ (KTO) substrate using two complementing techniques i.e., TEM and XRD, (2) to study growth mechanism of the BFO film, and (3) to demonstrate how to detect rhombohedral specific Bragg's reflection using XRD.

Rhombohedral specific Bragg's reflections are unambiguously found in nano beam electron diffraction (NBED) pattern as well as in x-ray reciprocal space mapping. This is consistent with structure factor calculation to reveal that the crystal structure within BFO film is rhombohedral. Epitaxial relationship found in NBED analysis indicates the BFO film grows in a manner that minimizes lattice mismatch with KTO substrate. Bright-field TEM and atomic resolution high angle annular dark field-STEM images revealed BFO/KTO interface is atomistically coherent with no sign of lattice strain relaxation. Atomistic models based on the epitaxial relationship indicate BFO film is under slight biaxial tensile stress (~0.35%) along in-plane direction. As a result, compressive uniaxial stress (~1.6%) is measured along out-of-plane direction of BFO film using XRD θ-2θ scan. This leads to Poisson's ratio of ~0.68.[1]

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[1] I.-T. Bae, T. Ichinose, M.-G. Han, Y. Zhu, S. Yasui & H. Naganuma, *Sci. Rep.* **8**, 893 (2018).