Structural analyses and first-principles simulation for new crystal symmetric $BiFeO_3$ grown on $LaAlO_3$ substrates

○Hiroshi Naganuma[1, 2], In-Tae Bae[3], András Kovács[4], Hong Jian Zhao[5], Jorge Íñiguez[5], Shintaro Yasui[6], Tomohiro Ichinose[1]

Tohoku Univ.[1], CNRS/Thales[2], Univ. NY[3], ER-C Peter Grünberg Inst.[4], LIST[5], Tokyo Tech.[6]

E-mail: naganumahiroshi1@gmail.com

New crystal and electronic structures of $BiFeO_3$ film grown on $LaAlO_3$ substrate are comprehensively studied using advanced transmission electron microscopy (TEM) technique[1)] combined with first-principles theory. Cross-sectional TEM images reveal the $BiFeO_3$ film consists of two zones with different crystal structures. [Fig. 1(a)] While zone II turns out to have rhombohedral $BiFeO_3$, the crystal structure of zone I matches none of $BiFeO_3$ phases reported experimentally or predicted theoretically. Detailed electron diffraction analysis combined with first-principles calculation allows us to determine that zone I displays a unique orthorhombic-like monoclinic new structure with space group of *C*m (= 8). The growth mechanism and electronic structure in zone I are further discussed in comparison with those of zone II. This study [2)] is the first to provide an experimentally validated complete crystallographic detail of a highly strained $BiFeO_3$ that includes the lattice parameter as well as the basis atom locations in the unit cell. [Fig. 1(b)]

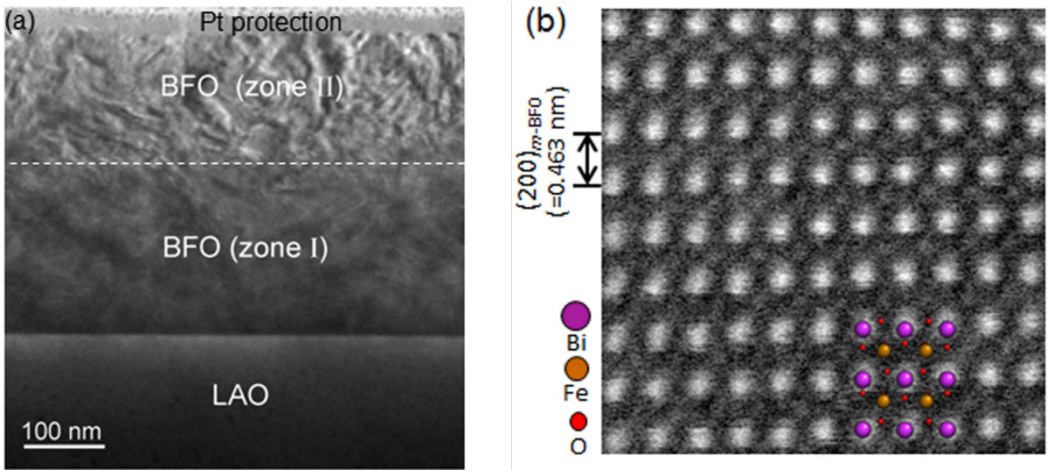

Figure 1 (a) TEM images of zone I (new BFO phase) and II (bulk BFO phase), (b) superposition of atomistic model of new BFO phase.

[1] In-T. Bae and H. Naganuma, Appl. Phys. Exp., **8**, 031501 (2015).

[2] In-T. Bae, A. Kovács, H. J. Zhao, J. Íñiguez, S. Yasui, T. Ichinose, H. Naganuma, Sci. Rep., **7**, 46498 (2017).

This research was partially funded by a Grant-in-Aid for Scientific Research (B) (No. 15H03548), S3IP at State University of NY at Binghamton, and JSPS Fellows No. JP16J01892. H. J. Z. and J. I. were funded by Luxembourg National Research Fund (Grant FNR/P12/4853155/Kreisel COFERMAT).