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Elucidation of crystal and electronic structures within highly strained BiFeO3 by transmission electron microscopy and first-principles simulation

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Crystal and electronic structures of ~380 nm $BiFeO_3$ film grown on $LaAlO_3$ substrate are comprehensively studied using advanced transmission electron microscopy (TEM) technique combined with first-principles theory. Cross-sectional TEM images reveal the $BiFeO_3$ film consists of two zones with different crystal structures. 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 an orthorhombic-like monoclinic structure with space group of Cm (=8). The growth mechanism and electronic structure in zone I are further discussed in comparison with those of zone II. This study 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.

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