Structural analyses and first-principles simulation for new crystal symmetric BiFeO$_3$ grown on LaAlO$_3$ substrates

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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 Cm (= 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.


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