講演題目：

Comprehensive crystal structure analysis for $BiFeO_3$ thin film using transmission electron microscopy

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講演要旨：

Great deal of recent interests in $BiFeO_3$ (BFO) has been triggered mostly by an article published in *Science*, 2003, which reported that BFO thin film can exhibit unusually high spontaneous polarization of ~60 μC/cm^2. Small change in lattice parameter induced by heteroepitaxial growth was argued as the mechanism for the high spontaneous polarization. Since knowledge about the crystal structure of BFO film is indispensable to properly interpret the high spontaneous polarization behavior found in thin film BFO, a number of studies have attempted to reveal the crystal structure of thin film BFO using x-ray scattering technique including reciprocal space mapping. While x-ray scattering is an excellent technique to investigate subtle changes in single crystal structure by focusing on local area in reciprocal space, it is difficult to acquire a wide range of reciprocal space information which is essential to properly interpret crystal structure overall. On the other hand, transmission electron microscopy (TEM) technique that makes use of 200 kV electron beam can readily provide two-dimensional reciprocal lattice information up to Q (scattering vector)=220 nm^{-1}, which is highly useful to evaluate overall crystal structure properly.

In this presentation, detailed crystal structure analysis of single crystalline BFO films grown on $SrTiO_3$ substrate with two different thicknesses, i.e., 30nm and 3nm, is performed using cross-sectional TEM technique from multi BFO zone axes for comprehensive crystal structure analysis.

As a result, it was found that nano-beam electron diffraction patterns combined with structure factor calculations and high-resolution transmission electron microscopy images unambiguously revealed that $BiFeO_3$ thin layers grow with rhombohedral structure. No evidence of monoclinic and/or tetragonal distortion is found. The rhombohedral $BiFeO_3$ thin layer is found to grow onto $SrTiO_3$ by maintaining an epitaxial relationship as follow:

(1) [241] of BFO // [010] of STO ; $(20\bar{4})$ of BFO // (200) of STO (along $[010]_{STO}$),

(2) [211] of BFO // [011] of STO ; $(10\bar{2})$ of BFO // (200) of STO (along $[011]_{STO}$).

Small lattice mismatch (<2.5 %) introduced at BFO/STO interface is considered to be the reason of the epitaxial relationships. NBED combined with SF analyses are proved to be useful to investigate crystal structure and its growth mechanism for BFO thin film.