Joint CQSE and CASTS Seminar

Weekly Seminar
Jun. 3, 2016 (Friday)

TIME Jun. 3, 2016, 14:30 ~ 15:30
TITLE Theoretical Study on The Oxygen Octahedral Tilt Domain Walls in Bismuth Ferrite
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Abstract

The multiferroics of Bismuth Ferrite ($BiFeO_3$, BFO) at room temperature make BFO an interesting material to scientists and engineers in very wide applications like piezoelectricity, photovoltaics, information storage devices, and even spintronics. BFO natural ground state possesses R3c rhombohedral symmetry with G-type antiferromagnetic arrangement and remnant polarization beyond 50μC/cm^2 along the directions perpendicular to {111} planes at room temperature. Its inherent ferroelectric polarization, ferromagnetic moments, and oxygen octahedral tilting actually offer the degrees of freedom for forming various types of domain walls. Recently the observed enhanced conductivity at ferroelectric domain walls,[1] vortex cores,[2] and abnormal photovoltaic effect crossing ferroelectric domain walls[3] have invoked scientists' attention to investigate the underlying mechanism of those phenomena. Domain wall engineering for possible applications of BFO and other perovskites via electric, magnetic fields, strain, doping and defects controls are also active directions in looking for fantastic functional devices.

Not long ago A. Lubk *et al.* have done the theoretical modeling to offer basic understanding of the enhanced conductivity crossing the ferroelectric domain walls.[4] However, the domain walls raised from the phase changing of oxygen octahedral tilt, which we found also have strong effects to the BFO conductivity were not addressed in literatures for the reasons of higher formation energy in theory and also not visible positions of oxygen atoms in measurements replying on Z-contrast. Via density functional theory calculations, we have successfully modeled the oxygen octahedral tilt domain walls along various directions and also some ferroelectric domain walls. I will show the differences between those domain walls in terms of formation energies, physical parameters, conduction and valence bands shifting, and local charge accumulation. And then I will give some comments on the existence of oxygen

octahedral tilt domain walls and also what may be observed in contrast to ferroelectric domain walls.

[1] J. Seidel *et al*., Nature Mater. **8**, 229 (2009).

[2] N. Balke *et al.*, Nature Physics **8**, 81 (2012).

[3] A. Bhatnagar, A. R. Chaudhuri, Y. H. Kim, D. Hesse, and M. Alexe, Nature Comm. **4**, 2835 (2013).

[4] A. Lubk, S. Gemming, and N. A. Spaldin, Phys. Rev. B **80**, 104110 (2009).