Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

First-principles study of the effect of oxygen vacancies around the 180° ferroelectric domain walls of tetragonal $PbTiO_3$ HOE-CHEOL SONG, HYE JUNG KIM, YOUNG-HAN SHIN*, University of Ulsan — People have extensively studied the dynamics of ferroelectric materials to apply them to nonvolatile memory devices. One of the issues in ferroelectric random access memory is the fatigue effect, which results from the presence of oxygen vacancy. Many cycles of polarization switching increase the density of oxygen vacancy around ferroelectric domain walls, and it makes the ferroelectric energy barrier higher to slow down the switching rate. In this presentation, we examine the domain dynamics around the 180° ferroelectric domain walls of tetragonal $PbTiO_3$ with and without the oxygen vacancy by using the first-principles calculations. We estimate the energy barriers of several possible reaction paths with the nudged elastic band method. Compared to the oxygen vacancy far away from domain walls, the oxygen vacancy around ferroelectric domain walls tends to be thermodynamically stable with lower energy barriers.Finally, we expect that by controling of oxygen vacancy density around the ferroelectric domain wall could be the solution for solving fatigue problem in ferroeletric materials.

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Date submitted: 14 Nov 2014 Electronic form version 1.4