Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Identification of Mn site in Pb(Zr,Ti)O_3 A. BOONCHUN[1], M.F. SMITH, S. RUJIRAWAT, B. CHERDHIRUNKORN, S. LIMPIJUMNONG, School of Physics, Suranaree University of Technology, Thailand — The impurity Mn in $PbTiO_3$ and $PbZrO_3$ has been studied by mean of first-principles spin density functional theory.[1] It is found that the Mn atom energetically prefers to substitute on the Ti/Zr site over other sites (i.e., Pb site, O site or interstitial) under all equilibrium growth conditions. The calculations predict that a majority of Mn atoms substitute for Ti/Zr and have neutral-charge state each with a total electron spin of $M_z = 3/2$. This prediction is supported by the combination of x-ray absorption near edge structure (XANES) experiment and first-principles simulation of the spectrum. [2] The measured XANES of the Mn-doped Pb(Ti,Zr)O_3 within the concentration range of 0.5 - 2.0 at.% yield the exact same features, indicating that the location of Mn in the crystal is independent of Mn concentration. The measured XANES is consistent with the partial density of states simulation of Mn atom on the Ti/Zr site and inconsistent with the simulations of Mn atom on other sites.
[1] A. Boonchun, M. F. Smith, B. Cherdhirunkorn, and S. Limpijumnong, J. Appl. Phys. 101, 043521 (2007). [2] S. Limpijumnong, S. Rujirawat, A. Boonchun, M.F. Smith, B. Cherdhirunkorn, Appl. Phys. Lett. 90, 103113 (2007).

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Date submitted: 26 Nov 2007 Electronic form version 1.4