Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Visable-Deep UV Dielectric Functions and Electronic Band Structure of Lead Zirconate Titanate Thin Films HOSUN LEE, T.D. KANG, Kyung Hee Univ., Y.S. KANG, S.-J. CHO, H. MORKOC, Virginia Commonwealth Univ., J. LI, S.-H. WEI, NREL, P.G. SNYDER, Univ. of Nebraska, Lincoln — We measure pseudodielectric functions in the visible-deep ultraviolet spectral range of $Pb(Zr_xTi_{1-x})O_3$ (x=0.2, 0.56, 0.82) (PZT), $Pb_{0.98}Nb_{0.04}(Zr_{0.2}Ti_{0.8})_{0.96}O_3$,$Pb_{0.91}La_{0.09}(Zr_{0.65}Ti_{0.35})_{0.98}O_3$, and$Pb_{0.85}La_{0.15}Ti_{0.96}O_3$ films. Using a parametric optical constant model, we estimate the dielectric functions (ε) of the perovskite oxide thin films. Taking the second derivative of the fitted layer dielectric functions and using the standard critical point model, we determine the parameters of the critical points. In the second derivative spectra, the lowest band gap energy peak near 4 eV is fitted as a double peak for annealed PZTs due to perovskite phase. As-grown PZTs have mainly pyrochlore phase and the lowest band gap peak is fitted as a single peak. We also examine the effect of dopants La and Nb, which substitute at Pb and Zr (Ti) sites, respectively. We found three band gaps E_a ($\sim$3.9eV), E_b ($\sim$4.5 eV)and E_c ($\sim$6.5eV) in the orderof increasing energy. The E_a and E_b band gap energies were not sensitive to Zr composition. We discuss the change of critical point (CP) parameters for PZTs in comparison to the band structure calculations based on local-density-approximation. The near-constancy of the lowest band gap energy independent of Zr composition is consistent with the band calculations.

Hosun Lee
Kyung Hee University

Date submitted: 01 Nov 2005 Electronic form version 1.4