Links Between Defect Chemistry, Conduction, and Lifetime in Heavily Nb Doped Lead Zirconate Titanate Films

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Phase pure PbZr0.52Ti0.48O3 (PZT) films with up to 13 mol. % Nb were prepared on Pt-coated Si substrates using chemical solution deposition; charge compensation for Nb was accomplished by reducing the concentration of lead in the film. For high Nb doping levels, (1) superoxidation of the PZT film surface makes the PZT/Pt interface more p-type and, hence reduces electron injection over the Schottky barrier, (2) the bulk charge transport mechanism changes from electron trapping by Ti4. to hole migration between lead vacancies, and (3) the ionic conductivity due to migration of oxygen vacancies decreases. For 6 mol:% Nb, electrical degradation was controlled via field-induced accumulation of oxygen vacancies near the cathode, which, in turn, leads to Schottky barrier lowering and electron trapping by Ti4.. In phase pure 13 mol. % Nb doped PZT films, on the other hand, the increase in the leakage current during electrical degradation was dominated by hole migration between lead vacancies (2.[V"Pb]~[h*]. A much lower lifetime and drastic increase in the leakage current upon electrical degradation was observed in mixed phase PNZT films, which was attributed to (1) a more electrically conductive pyrochlore phase and (2) a high concentration of lead vacancies.