Enhanced Piezoelectricity in PbTiO$_3$/BaTiO$_3$ Superlattices

T. YUSUFALY, Rutgers University, B. ZIEGLER, University of Geneva, V.R. COOPER, Oak Ridge National Laboratory, S.J. CALLORI, J. SINSHEIMER, Stony Brook University, K.M. RABE, P. CHANDRA, Rutgers University, M. DAWBER, Stony Brook University — First-principles calculations by Cooper and Rabe predict an enhancement of the piezoelectric coefficient ($d_{33}$) in PbTiO$_3$/BaTiO$_3$ (PTO/BTO) superlattices for intermediate values of PTO concentration. PTO/BTO superlattices have been fabricated using an off-axis RF magnetron sputtering technique, enabling x-ray diffraction, electrical measurements and atomic force microscopy on this system. The experimental results agree with the calculated polarization, tetragonality and enhanced piezoelectricity as a function of PTO concentration. Additional first-principles calculations indicate that the enhancement in $d_{33}$ is more pronounced in shorter-period superlattices. By applying a Landau-Devonshire model to this system, we find that the enhanced piezoelectricity is due to the combination of a bulk effect associated with the presence of finite electric fields in each layer and interfacial effects. Implications of our results for future experiments are discussed.

T. Yusufaly
Rutgers University

Date submitted: 13 Dec 2011