Compositionally Graded Ferroelectrics as Wide Band Gap Semiconductors: Electrical Domain Structures and the Origin of Low Dielectric Loss

I. B. Misirlioglu,[1,a] and S. P. Alpay [2,3]

[1] *Faculty of Engineering and Natural Sciences*
Sabanci University, Tuzla/Orhanli 34956 Istanbul, Turkey
[2] *Department of Materials Science and Engineering and Institute of Materials Science*
University of Connecticut, Storrs, CT 06269 – USA
[3] *Department of Physics, University of Connecticut, Storrs, CT 06269 – USA*

[a] author to whom correspondence should be addressed, burc@sabanciuniv.edu

---

Abstract

Functional materials with compositional gradients exhibit unique characteristics that are different from the components comprising the structure. Graded ferroelectrics are very good examples to such materials where a systematic variation in composition is introduced along the thickness of a thin film heterostructure. Such structures display interesting properties including the disappearance of the dielectric anomaly at the ferroelectric-paraelectric transition that is otherwise observed in monolayer ferroelectrics, a strong internal ("built-in") electric field, low dielectric loss, and an almost temperature insensitive dielectric tunability. We present here a theoretical study to understand some interesting properties of graded ferroelectrics by treating these as wide band gap semiconductors. Such an approach allows us to address the effect of impurities/dopants. We specifically analyze compositionally graded (001) heteroepitaxial $(Pb,Sr)TiO_3$ films between Pt electrodes on (001) $SrTiO_3$. Our analysis shows that a single-domain state could be stabilized in the presence of space charges whereas intrinsic stacks display wedge-like electrical domain patterns. The computations also provide an explanation as to why graded ferroelectrics should have lower dielectric losses and lower leakage currents compared to monolayer ferroelectrics. We attribute this to the carrier depletion in the layers due to built-in electric fields resulting from the polarization mismatch.