Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Dependence of Polarization and Dielectric response on Epitaxial Strain in $(Ba_xSr_{1-x})TiO_3$ Ultrathin Films from First-Principles
SAAD BIN-OMRAN, King Saud University — A first-principles-derived schemes is used to use a first-principles-derived technique to construct the temperature-versus-misfit strain phase diagrams for the whole BST composition rang (i.e., x=0.00,0.20,0.40,0.60,0.80,1.00). Moreover, we investigate the dependence of their dielectric and ferroelectric properties on the strain and the concentration. Our results reveal that the predicated phase diagrams show a topology similar to those calculated by Shirokov et. al. Phy. Rev. B. **79** 144118 (2009) with quantitative discrepancies that will be revealed and explained. Our results also indicate that in-plane strain increases (respectively, decreases) the in-plane (respectively, out-of-plane) dielectric constants. Furthermore, the out-of-plane component of dielectric permittivity ε_{33} enhances with lowering x in $(Ba_xSr_{1-x})TiO_3$ films. We hope that our results will be benefits to many scientists and will lead to new strategies for material design.

Saad Bin-Omran
King Saud University

Date submitted: 18 Nov 2011 Electronic form version 1.4