Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Dielectric Relaxation in (BiFeO3)1-x-(KNbO3)x solid solutions
RADHE AGARWAL, Univ. of Puerto Rico, FAN ZHENG, Univ. of Pennsylvania, YOGESH SHARMA, Univ. of Puerto Rico, ANDREW RAPPE, Univ. of Pennsylvania, RAM KATIYAR, Univ. of Puerto Rico — We have studied structural, optical and dielectric properties of (BiFeO3)x-(KNbO3)1-x (BFO-KNO) solid solutions with a combination of first principle calculations and experimental methods. Theoretically, we have used density functional theory to predict optical band gap in 40 atom pseudocubic ABO3 type (BFO)1-x-(KNO)x [x=0 to 1] supercells. We observed a rhombohedral to orthorhombic type distortion as the doping concentration increased from 0 to 1. For x=0.05, we observed a random off center displacements of A-site atoms (Bi, K) from the corresponding oxygen cage (BO6). Such type of behavior can be associated with disruption in long range polar orderings and thus creating short range (nano) polar regions. To further investigate the possibility of dielectric relaxation, we carried out temperature dependent dielectric spectroscopic measurements on (BFO)0.95-(KNO)0.05 bulk ceramics. We observed frequency dependent temperature of permittivity maximum (Tmax) around 540 K. Further, the frequency dispersion in dielectric constant and dielectric loss spectra, and a clear polarization hysteresis near room temperature were observed, which indicate relaxor behavior of (BFO)0.95-(KNO)0.05. Our study leads a way to develop lead free relaxor material, which can be used for various piezoelectric applications.

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Date submitted: 11 Nov 2016 Electronic form version 1.4