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Bulk photovoltaic effect in epitaxial (K, Nb) substituted BiFeO3 thin films RADHE AGARWAL, Univ. of Puerto Rico, FAN ZHENG, Univ. of Pennsylvania, YOGESH SHARMA, Univ. of Puerto Rico, SEUNGBUM HONG, 1) Argonne National Laboratory 2) KAIST, ANDREW RAPPE, Univ. of Pennsylvania, RAM KATIYAR, Univ. of Puerto Rico — We studied the bulk photovoltaic effect in epitaxial (K, Nb) modified BiFeO3 (BKFNO) thin films using theoretical and experimental methods. Epitaxial BKFNO thin films were grown by pulsed laser deposition (PLD). First, we have performed first principles density function theory (DFT) using DFT+U method to calculate electronic band structure, including Hubbard-Ueff (Ueff=U-J) correction into Hamiltonian. The electronic band structure calculations showed a direct band gap at 1.9 eV and a defect level at 1.7 eV (in a 40 atom BKFNO supercell), sufficiently lower in comparison to the experimentally observed values. Furthermore, the piezoforce microscopy (PFM) measurements indicated the presence of striped polydomains in BKFNO thin films. Angle-resolved PFM measurements were also performed to find domain orientation and net polarization directions in these films. The experimental studies of photovoltaic effect in BKNFO films showed a short circuit current of 59 micro amp/cm2 and open circuit voltage of 0.78 V. We compared our experimental results with first principles shift current theory calculations of bulk photovoltaic effect (BPVE).The synergy between theory and experimental results provided a realization of significant role of BPVE in order to understand the photovoltaic mechanism in ferroelectrics.

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