Experimental Characterization And Theoretical Analysis Of Highly Tunable Paraelectric Perovskite Thin Films*

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The nonlinear dielectric responses of one axis oriented polycrystalline $(Ba_{1-x}Sr_x)TiO_3$ (BST) thin films are studied by adjusting the film lattice constant. BST films were deposited by reactive magnetron rf sputtering on epitaxial quality Pt electrodes. The various degree of nonlinearity of the relative dielectric constants (i.e., voltage tunabilities) of the BST films, accompanied with relatively stable dependence of dielectric loss factors (tan δ) under moderate to high electric fields were correlated with the growth conditions-induced cubic lattice distortions of the BST layer in Metal/Ferroelectric/Metal (MFM) capacitor structures. A 2.5 times increase in the relative dielectric constant and voltage tunability of the optimized Pt/BST/Pt stacks was observed with some variation of deposition condition during the growth of the BST layer while keeping parameters such as deposition temperature, the Ba/(Ba+Sr) ratio, film thickness, substrate type, electrode material, etc. the same. The observed increase of the voltage tunability was achieved concurrently without any deterioration or accompanied with additional improvement of other dielectric properties, e.g.: tan δ–voltage symmetry and stability, leakage current behavior, breakdown voltage, temperature dependence of the capacitance and temperature dependence of the dielectric tunability. To clarify the effects of the deposition conditions on structural and electrical properties of BST thin films, we performed theoretical calculations based on the density functional theory (DFT). In this presentation we discuss the phenomenological relationship between small structural distortions, residual bond strain, bond-valence-sum parameters and the nonlinear dielectric properties of paraelectric perovskites.

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