Electronic supplementary information for the RSC Advances paper

Effect of insertion of low leakage polar layer on leakage current and multiferroic properties of BiFeO₃/BaTiO₃ multilayer structure

Savita Sharma^{1,3}, Monika Tomar², Ashok Kumar⁴, Nitin K. Puri³ and Vinay Gupta^{1*}

¹Department of Physics and Astrophysics, University of Delhi, Delhi, INDIA,

²Physics Department, Miranda House, University of Delhi, Delhi, INDIA,

³Department of Applied Physics, Delhi Technological University, Delhi, INDIA,

⁴CSIR-National Physical Laboratory, Dr. K.S. Krishnan Marg, Delhi, INDIA

Fig. S1 Schematic diagram of BiFeO₃/BaTiO₃ multilayers prepared on Silicon substrate



Fig. S2 C-V characteristics of BiFeO₃/BaTiO₃ multilayer structure having six stacking layers.



Fig. S2 represents the capacitance - voltage (C-V) characteristics of six layer BiFeO₃/BaTiO₃ structure. A little asymmetry was observed in the C-V curve due to the difference in the top (Au) and bottom (Pt) electrodes.

			BaTiO₃		BiFeO ₃			
	Lattice parameter		Stress modulus	c/a distortion	Lattice parameter		Stress modulus	c/a distortion
	a (Å)	c (Å)	(%)	ratio	a (Å)	c (Å)	(%)	ratio
2 layers	3.985	4.024	0.223	1.0097	5.492	13.423	3.201	2.4437
3 layers	4.372	4.061	0.694	0.9288	5.495	13.419	3.230	2.4420
4 layers	4.369	4.058	0.619	0.9288	5.530	13.548	2.300	2.4499
5 layers	4.385	4.080	1.165	0.9304	5.535	13.530	2.430	2.4444
6 layers	4.372	4.078	1.115	0.9327	5.424	13.315	3.980	2.4548
7 layers	4.598	4.095	1.537	0.8906	5.420	13.321	3.937	2.4577
Bulk	3.999	4.033		1.0085	5.876	13.867		2.3599

Table ST 1: Lattice parameters "a" and "c", c/a lattice distortion and stress modulus along c-axis in the BaTiO₃ and BiFeO₃ layers in BiFeO₃/BaTiO₃ multilayer structures.

The lattice parameters of BiFeO₃ and BaTiO₃ in multilayer thin film structures were calculated by Le-Bail fitting using Bruker Topas 3 software. The corresponding data reported for bulk BaTiO₃ and BiFeO₃ are also included in Table ST 1 for comparison. The values of lattice parameters a and c were estimated to be 4.372 Å and 4.078 Å for BaTiO₃ and 5.424 Å and 13.315 Å for BiFeO₃ respectively for the six layered BiFeO₃/BaTiO₃ system (Table ST 1). These values are slightly lower than the corresponding bulk values for BiFeO₃ and slightly greater in case of BaTiO₃ [JCPDS card No. 01-072-0138 and 01-072-2035], indicating the presence of stress in the BiFeO₃/BaTiO₃ multilayer structures prepared by PLD. The stress modulus in the BiFeO₃/BaTiO₃ multilayer thin film is obtained using equation: Stress = $(c_0-c)/c_0$ in %, where "c" is the respective lattice constant of BiFeO₃ or BaTiO₃ in deposited multilayer structure and " c_0 " is the corresponding bulk value.

	Ρ _r (μC/cm²)	P _s (µC/cm²)	2E _c (kV/cm)	Leakage current (A)	M _r (emu/cm³)	M₅ (emu/cm³)
2 layers	8.29	17.92	6.06	1.52 x 10 ⁻⁵	10.33	28.29
3 layers	13.40	29.46	6.49	2.51 x 10 ⁻⁶	13.45	37.67
4 layers	29.53	49.60	6.77	6.38 x 10 ⁻⁷	21.26	56.42
5 layers	45.72	64.47	11.18	1.62 x 10 ⁻⁷	32.98	86.88
6 layers	72.14	99.80	10.25	3.18 x 10 -8	35.32	94. 70
7 layers	15.96	26.25	11.11	5.16 x 10⁻ ⁶	15.79	42.36

 Table ST 2: Ferroelectric, ferromagnetic parameters and leakage current of BiFeO₃/BaTiO₃

 multilayer structures having different number of layers.