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

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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.