**Supplemental material:**

**Influence of Zn2+ doping on the morphotropic phase boundary in lead-free piezoelectric (1-x)Na1/2Bi1/2TiO3-xBaTiO3**

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# Supplemental material

Table S 1: Average grain size and variance of NBT-xBT and NBT-xBT-0.5 Zn samples.

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | **-5BT** | **-5.5BT** | **-6BT** | **-6.5BT** | **-7BT** | **-5BT-0.5 Zn** | **-5.5BT-0.5 Zn** | **-6BT-0.5 Zn** | **-6.5BT-0.5 Zn** | **-7BT-0.5 Zn** |
| **Grain size (μm)** | 2.1 | 1.4 | 1.7 | 1.2 | 1.2 | 14.7 | 15.6 | 9.4 | 14.1 | 13.8 |
| **Variance (μm)** | 2 | 0.8 | 0.8 | 0.7 | 0.7 | 5.5 | 6.6 | 4.4 | 6.5 | 5.9 |

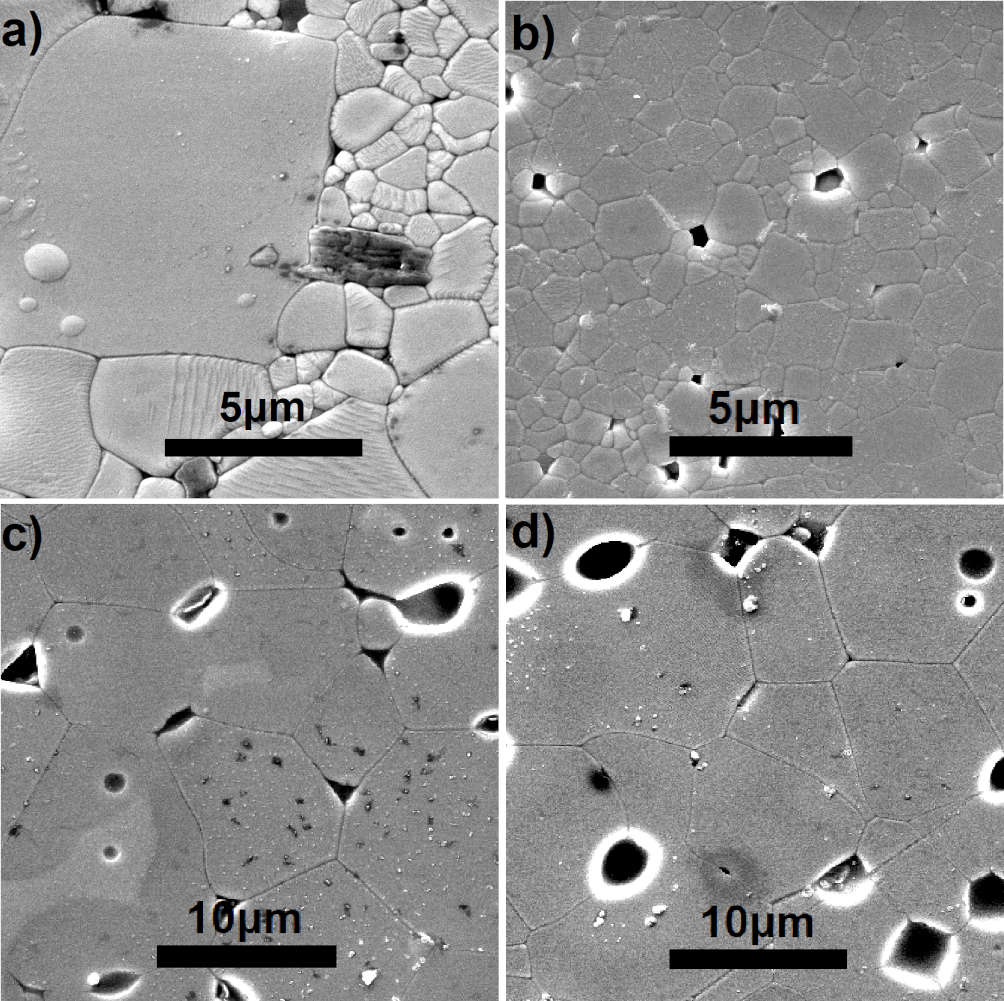


Figure S 1: Microstructures of the ground, polished and thermally-etched NBT-5BT (a), NBT-7BT (b), NBT-5BT-0.5 Zn (c) and NBT-7BT-0.5 Zn (d) samples.

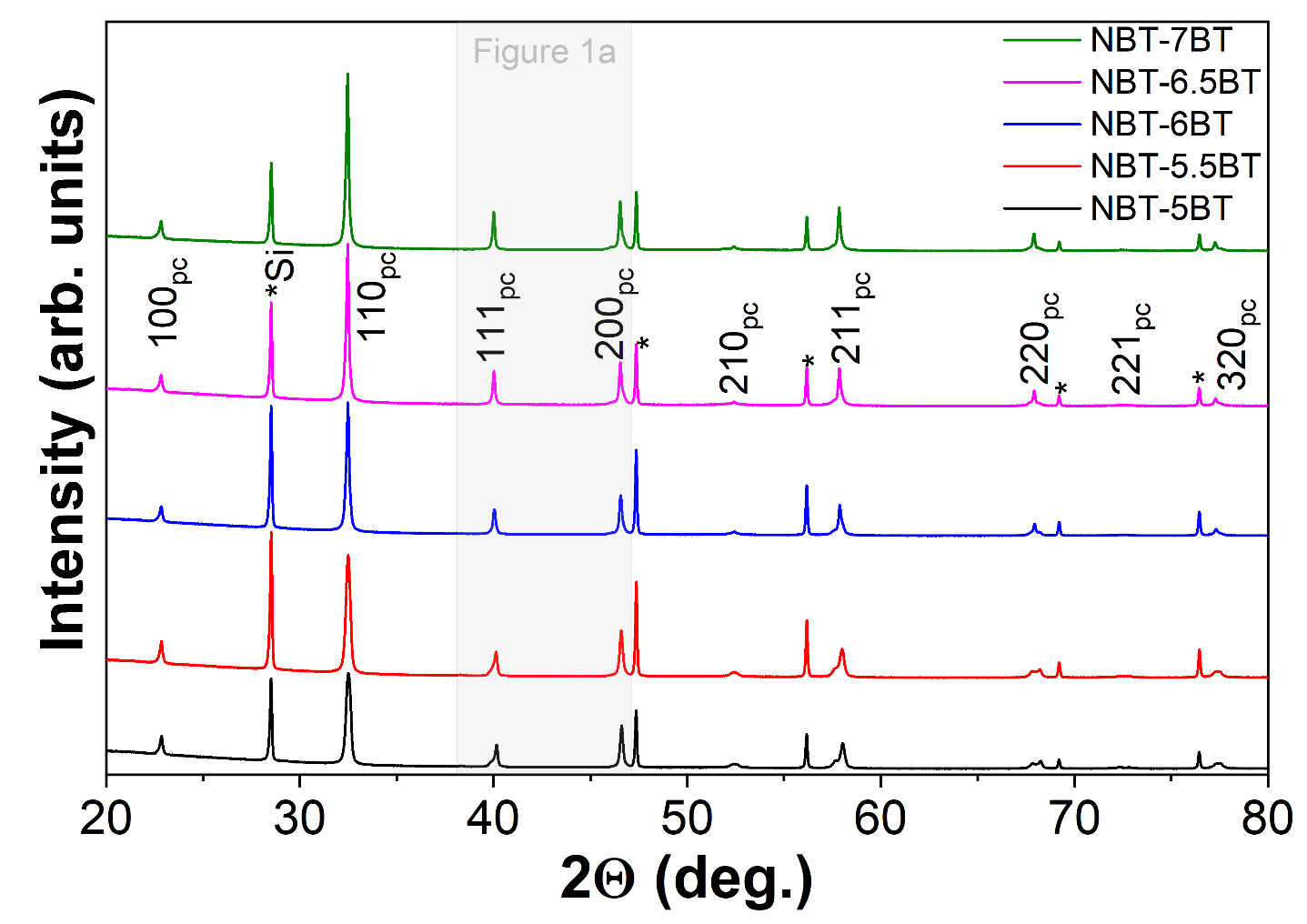


Figure S 2: X-ray diffraction profiles of (1-x)NBT-xBT with x=0.05, 0.055, 0.06, 0.065, 0.07. The NBT-BT powders were mixed with a silicon standard to get the instrumental parameters (Si peaks are marked with \*).

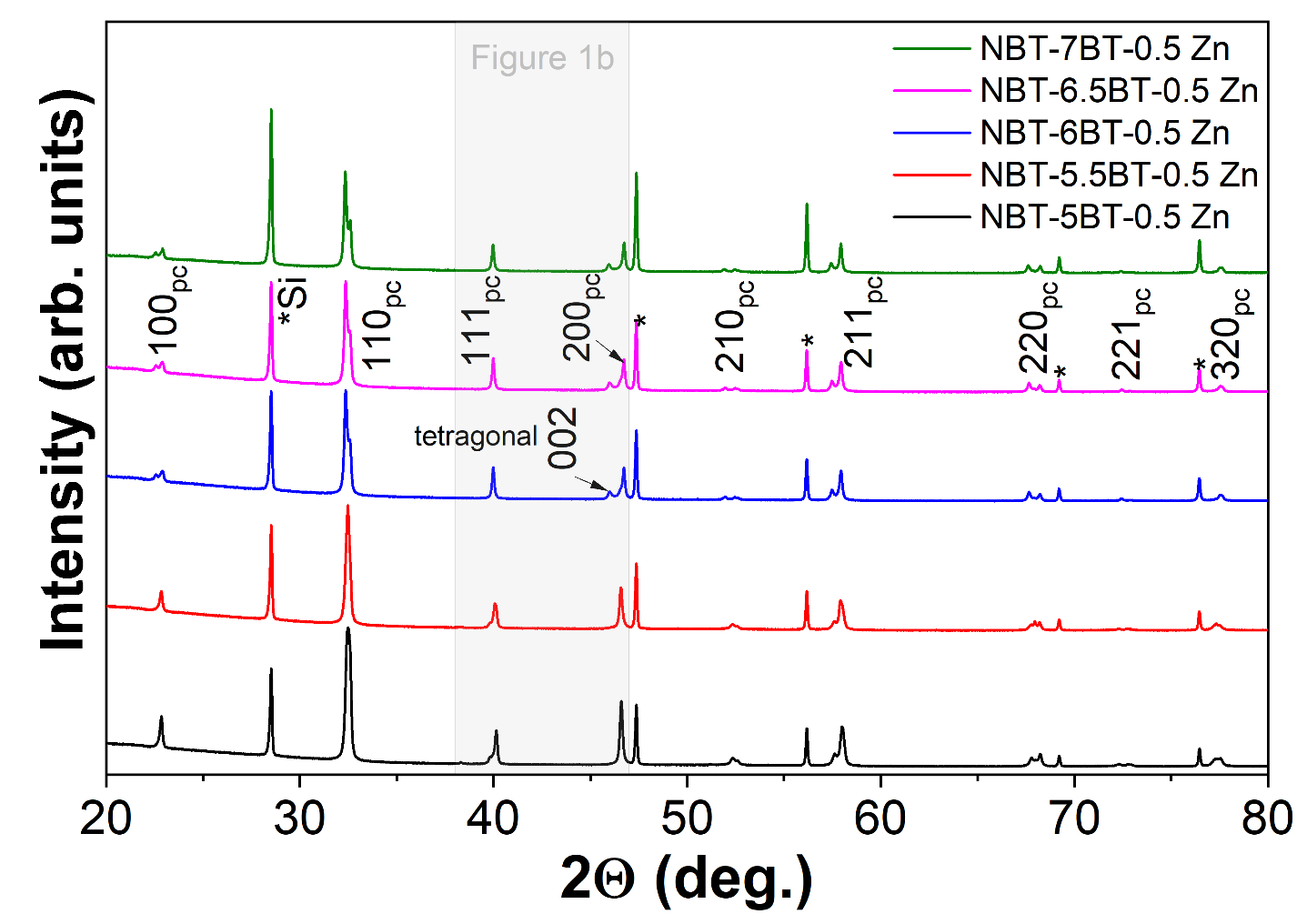


Figure S 3: X-ray diffraction profiles of (1-x)NBT-xBT-0.5 mol % Zn with x=0.05, 0.055, 0.06, 0.065, 0.07. An internal silicon standard was measured to get the instrumental parameters (Si peaks are marked with \*).

Table S : Detailed refinement data.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | ***R*3*c*** | |  | ***P*4*mm*** | | **Reliability factors** |
| **NBT-5BT** | a= 5.4999 (Å) c= 13.5773 (Å)  V= 59.28 | | a= 3.9003 (Å)  V= 59.34 |  | | Rp: 2.36 Rwp: 3.25 Rexp: 1.65 |
| **NBT-5.5BT** | a= 5.5033 (Å) c= 13.5739 (Å) V= 59.34 | | a= 3.9031 (Å)  V= 59.46 |  | | Rp: 3.08 Rwp: 5.24 Rexp: 1.54 |
| **NBT-6BT** | a= 5.5023 (Å) c= 13.5939 (Å) V= 59.40 | | a= 3.9038 (Å)  V= 59.49 | a= 3.8922 (Å) c= 3.9378 (Å) V= 59.65 | | Rp: 2.19 Rwp: 3.11 Rexp: 1.60 |
| Site x y z  Na 0.00000 0.00000 0.27582  Bi 0.00000 0.00000 0.27582  Ba 0.00000 0.00000 0.27582  Ti 0.00000 0.00000 0.02083  O 0.08893 0.35931 0.08330 | | Site x y z  Na 0.00000 0.00000 0.00000  Bi 0.00000 0.00000 0.00000  Ba 0.00000 0.00000 0.00000  Ti 0.50000 0.50000 0.50000  O 0.50000 0.50000 0.00000 | | | Site x y z  Bi 0.00000 0.00000 0.00000  Ba 0.00000 0.00000 0.00000  Na 0.00000 0.00000 0.00000  Ti 0.50000 0.50000 0.45432  O 0.50000 0.50000 -0.15000  O 0.50000 0.00000 0.40000 | |
| **NBT-6.5BT** |  | | a= 3.9053 (Å)  V= 59.56 | a= 3.8932 (Å) c= 3.9339 (Å) V= 59.63 | | Rp: 2.29 Rwp: 3.23 Rexp: 1.57 |
| **NBT-7BT** |  | | a= 3.9058 (Å)  V= 59.59 | a= 3.8947 (Å) c= 3.9350 (Å) V= 59.69 | | Rp: 2.31 Rwp: 3.50 Rexp: 1.61 |
| **NBT-5BT**  **-0.5 Zn** | a= 5.5013 (Å) c= 13.5908 (Å) V= 59.37 | | a= 3.8998 (Å)  V= 59.31 |  | | Rp: 2.47 Rwp: 3.76 Rexp: 1.59 |
| **NBT-5.5BT**  **-0.5 Zn** | a= 5.5023 (Å) c= 13.5987 (Å) V= 59.43 | | a= 3.9023 (Å)  V= 59.43 | a= 3.8907 (Å) c= 3.9385 (Å) V= 59.62 | | Rp: 2.21 Rwp: 3.22 Rexp: 1.64 |
| **NBT-6BT**  **-0.5 Zn** | a= 5.5043 (Å) c= 13.5989 (Å) V= 59.47 | | a= 3.9048 (Å)  V= 59.54 | a= 3.8895 (Å) c= 3.9467 (Å) V= 59.71 | | Rp: 2.08 Rwp: 3.09 Rexp: 1.63 |
| **NBT-6.5BT**  **-0.5 Zn** |  | | a= 3.9051 (Å)  V= 59.55 | a= 3.8903 (Å) c= 3.9475 (Å) V= 59.75 | | Rp: 1.87 Rwp: 2.79 Rexp: 1.64 |
| **NBT-7BT**  **-0.5 Zn** |  | | a= 3.9062 (Å)  V= 59.6 | a= 3.8899 (Å) c= 3.9520 (Å) V= 59.8 | | Rp: 2.63 Rwp: 4.49 Rexp: 1.72 |

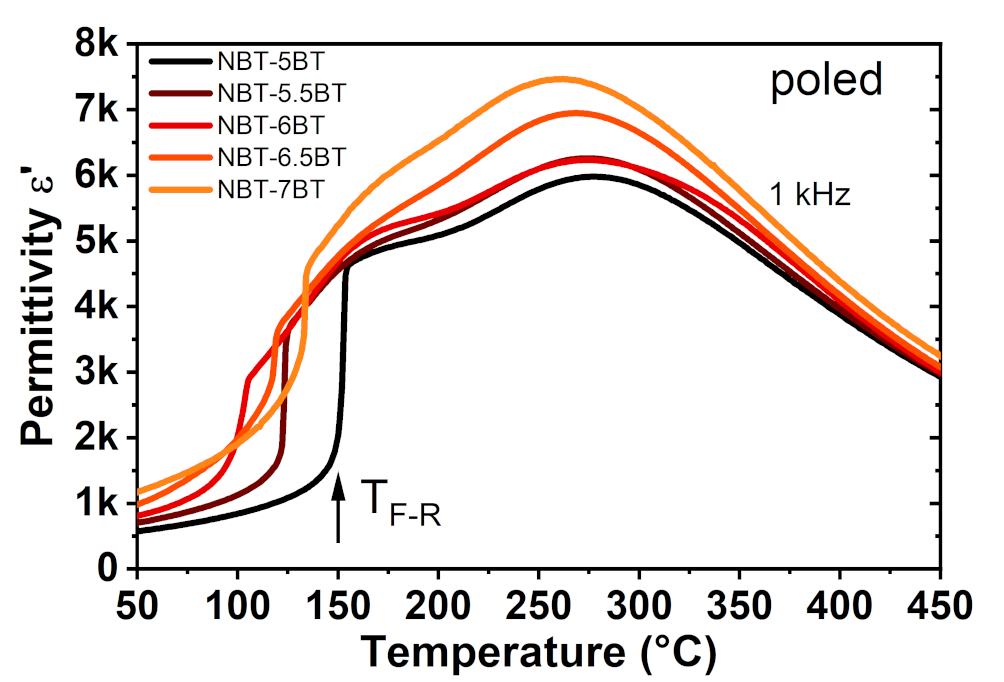


Figure S : Permittivity vs. temperature at 1 kHz AC-field from NBT-5BT to NBT-7BT. All samples are measured in poled state to evaluate TF-R.

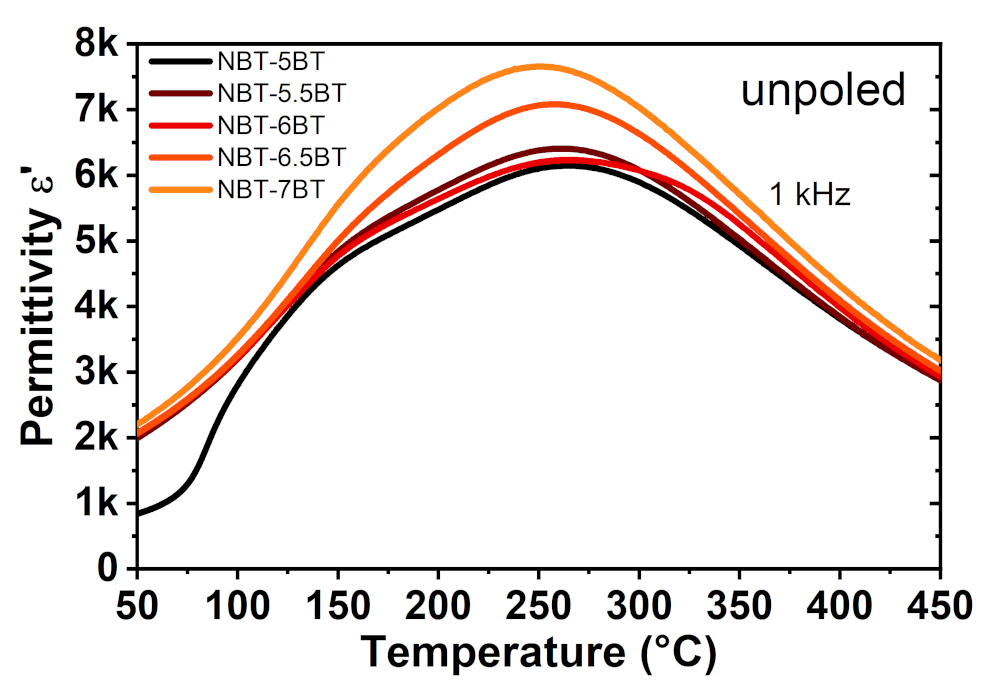


Figure S : Permittivity vs. temperature at 1 kHz AC-field from NBT-5BT to NBT-7BT. All samples are measured in unpoled state.

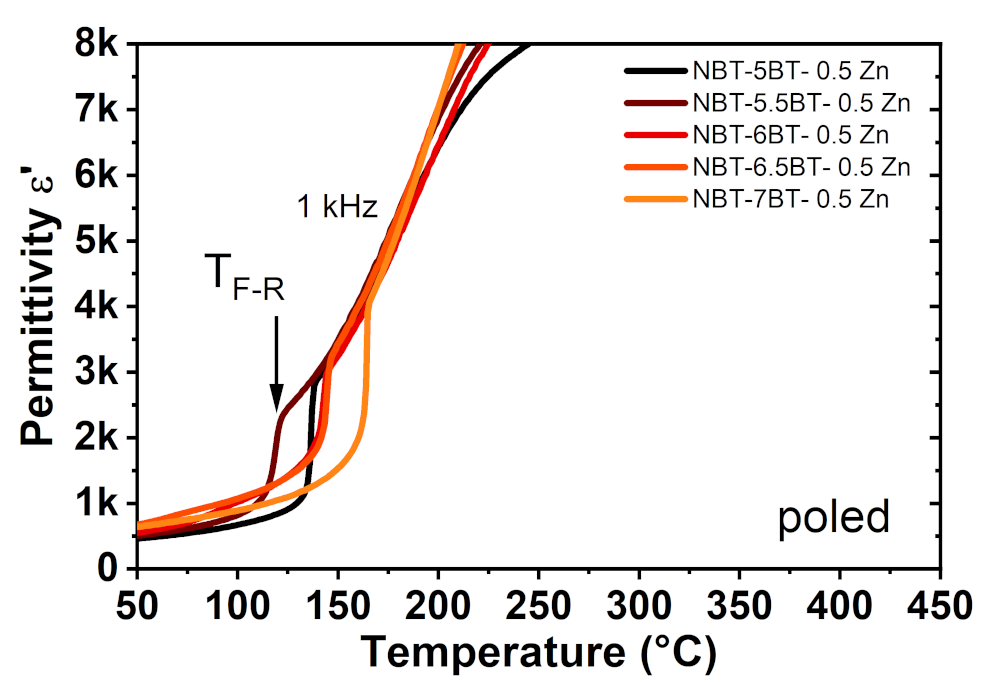


Figure S : Permittivity vs. temperature at 1 kHz AC-field from NBT-5BT-0.5 Zn to NBT-7BT-0.5 Zn. All samples are measured in poled state to evaluate TF-R.

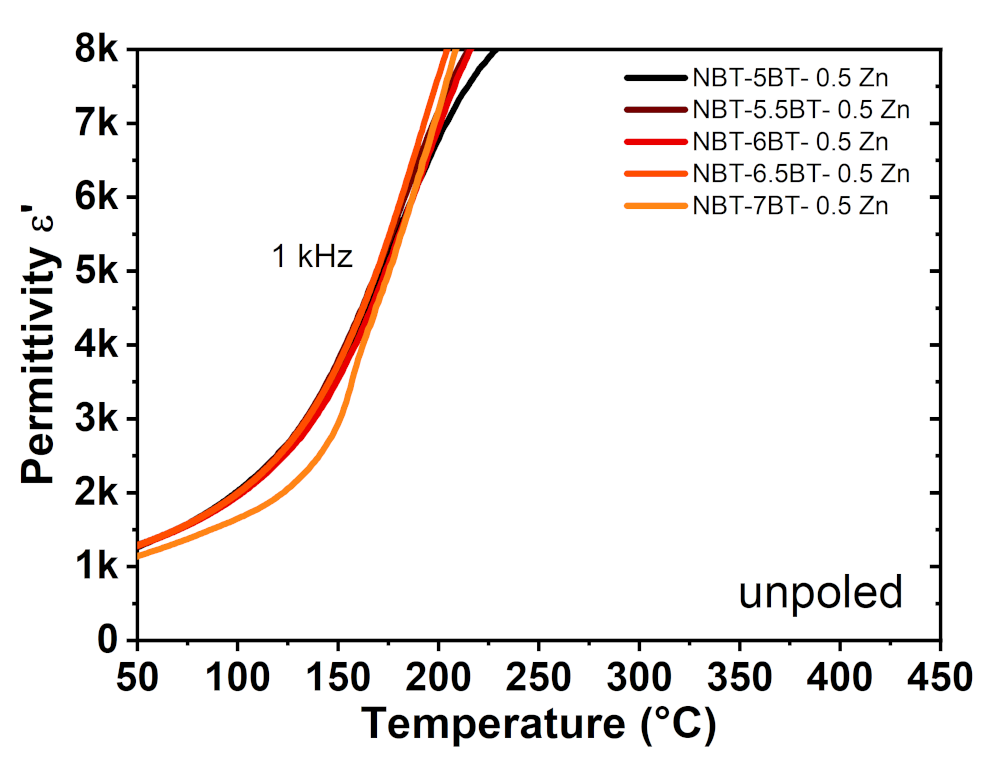


Figure S : Permittivity vs. temperature at 1 kHz AC-field from NBT-5BT-0.5 Zn to NBT-7BT-0.5 Zn. All samples are measured in unpoled state.