

Supplementary Information

Enhanced tetragonality and large negative thermal expansion in a new Pb/Bi-based perovskite ferroelectric of $(1-x)\text{PbTiO}_3-x\text{Bi}(\text{Zn}_{1/2}\text{V}_{1/2})\text{O}_3$

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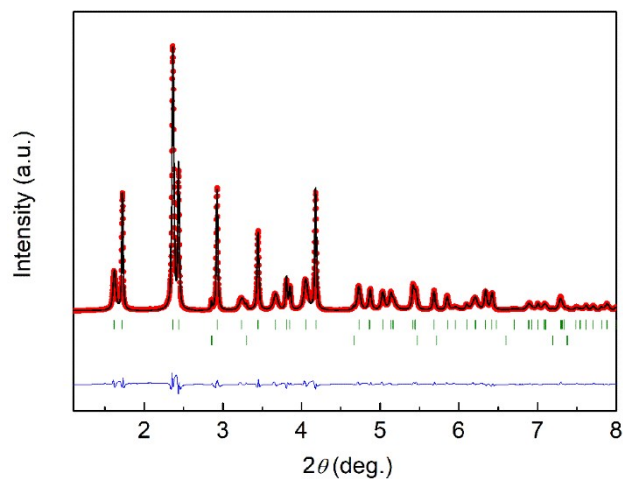


Figure S1. Rietveld full profile refinement of SXRD patterns of tetragonal 0.9PT-0.1BZV at room temperature. Observed (red, solid circles), calculated (black line), and their difference profiles (bottom line) are shown. The Bragg reflection positions are indicated by the green ticks. Note that a minority phase of Au derived from the gold capsule for the high-pressure experiment was observed for all investigated samples.

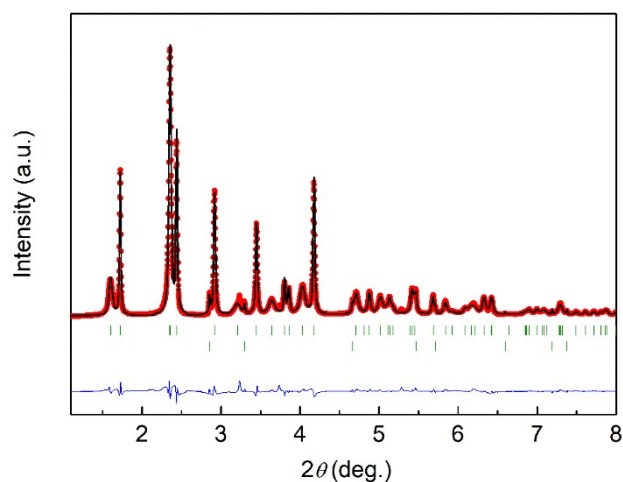


Figure S2. Rietveld full profile refinement of SXRD patterns of tetragonal 0.8PT-0.2BZV at room temperature. Observed (red, solid circles), calculated (black line), and their difference profiles (bottom line) are shown. The Bragg reflection positions are indicated by the green ticks.

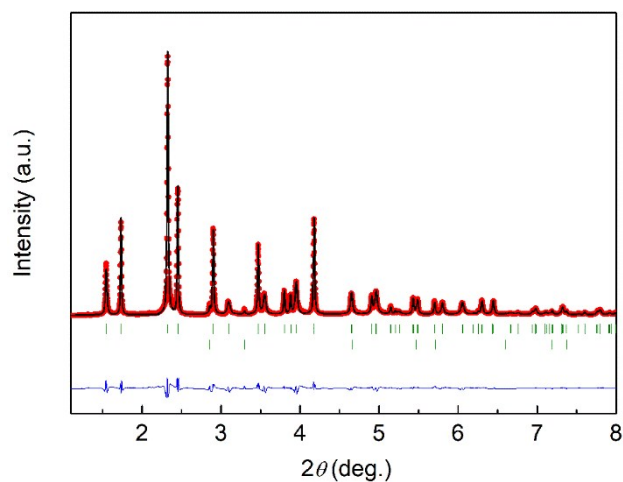


Figure S3. Rietveld full profile refinement of SXRD patterns of tetragonal 0.7PT-0.3BZV at room temperature. Observed (red, solid circles), calculated (black line), and their difference profiles (bottom line) are shown. The Bragg reflection positions are indicated by the green ticks.

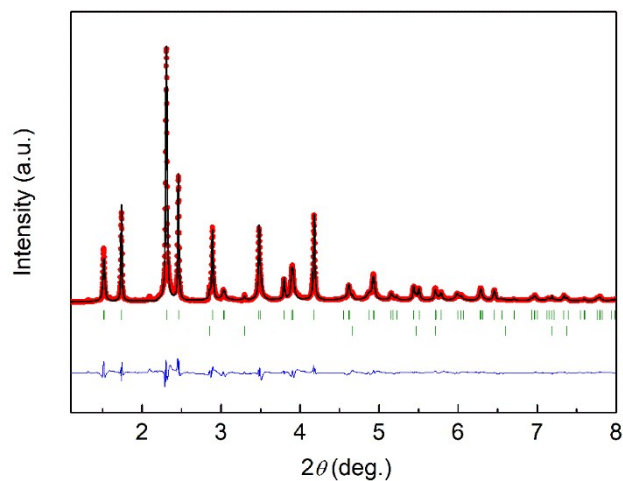


Figure S4. Rietveld full profile refinement of SXRD patterns of tetragonal 0.6PT-0.4BZV at room temperature. Observed (red, solid circles), calculated (black line), and their difference profiles (bottom line) are shown. The Bragg reflection positions are indicated by the green ticks.

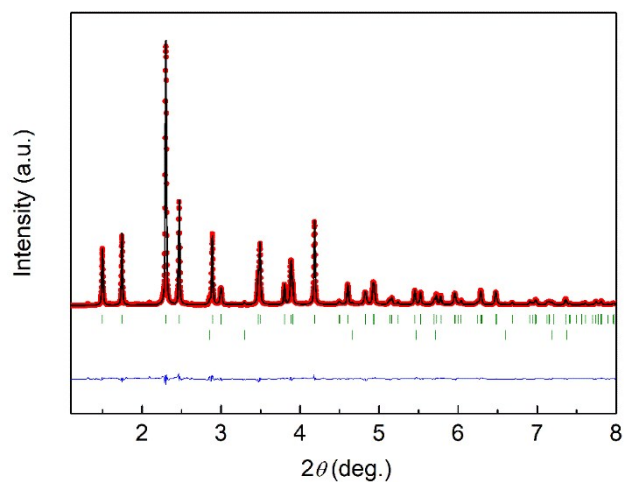


Figure S5. Rietveld full profile refinement of SXR D patterns of tetragonal 0.5PT-0.5BZV at room temperature. Observed (red, solid circles), calculated (black line), and their difference profiles (bottom line) are shown. The Bragg reflection positions are indicated by the green ticks.

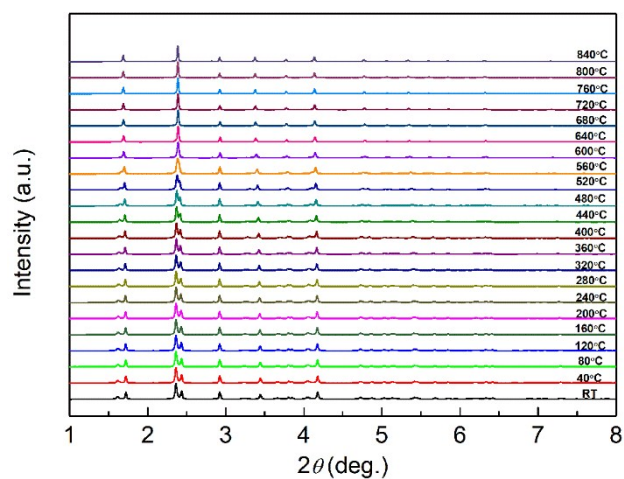


Figure S6. Temperature dependence of SXR D patterns of 0.9PT-0.1BZV with an interval of 40 °C.

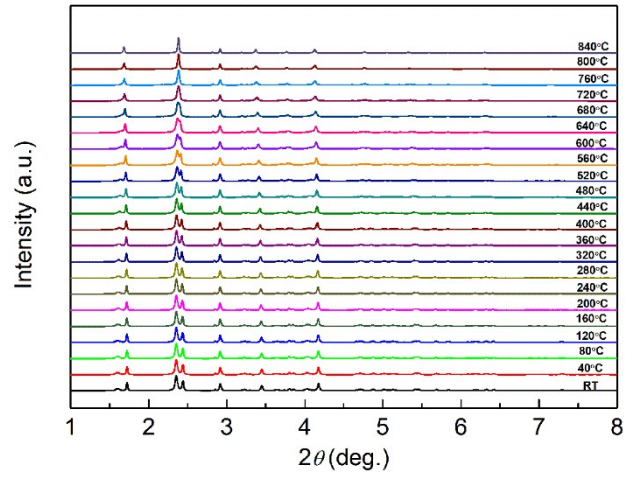


Figure S7. Temperature dependence of SXRD patterns of 0.8PT-0.2BZV with an interval of 40 °C.