Supplementary Information for

Phase transition and piezoelectricity of sol-gel-processed Sm-doped BiFeO₃ thin films on Pt(111)/Ti/SiO₂/Si substrates

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The XRD patterns were analyzed with Rietveld refinement.¹ It should be addressed that since the intensity of Pt bottom electrode is extremely strong, about 3 orders of magnitude higher than BiFeO₃ thin films, different space groups of BiFeO₃ make little difference during refinement. To eliminate this influence, the region with peak of Pt was excluded during the refinement. The refinements for all the samples were carried out with three basic space groups as have been reported in the rare-earth doped BiFeO₃ system, i.e., *R3c*, *Pbam* and *Pnma* respectively.^{2, 3} For *x*=0 and 0.05, the patterns were found to fit well with *R3c* structure. For the compositions *x*=0.10 and 0.15, which may be the underlying MPB, we further tried the *R3c+Pbam* and *Pbam+Pnma* structural models. According to fitting factors R_w and χ^2 , the refinement of *x*=0.10 match well with *R3c* (68.55%) + *Pbam* (31.45%), confirming the early analysis of *R* and *O* phase coexistence. For the refinement of *x*=0.15, *Pbam*(10.15%) + *Pnma*(89.85%) model gave the smallest fitting factors. The detailed refinement results are shown in Table S1 and are plotted in Fig. S1.

Composition	Crystal structure	Space group	Lattice parameter	Fitting factors
<i>x</i> =0	Rhombohedral	<i>R</i> 3 <i>c</i> :H	<i>a</i> =5.5355(2)Å <i>c</i> =13.7181(0)Å Volume=364.03Å ³	$R_{\rm w}$ =7.56 χ^2 =4.56
<i>x</i> =0.05	Rhombohedral	<i>R3c</i> :H	<i>a</i> =5.5526(0)Å <i>c</i> =13.7274(7)Å Volume=366.53 Å ³	$R_{\rm w}$ =5.60 χ^2 =2.52
<i>x</i> =0.10	Rhombohedral	<i>R</i> 3 <i>c</i> :H (68.55%)	<i>a</i> =5.5580(1)Å <i>c</i> =13.7664(7)Å Volume=368.29 Å ³	$R_{\rm w}$ =5.78 χ^2 =2.41
	Orthorhombic	<i>Pbam</i> (31.45%)	<i>a</i> =5.5971(9)Å <i>b</i> =11.1511(4) Å <i>c</i> =7.8150(2)Å Volume=487.77 Å ³	
<i>x</i> =0.15	Orthorhombic	Pbam (10.15%)	<i>a</i> =5.5629(0)Å <i>b</i> =11.1409(9)Å <i>c</i> =7.8107(2)Å Volume=484.08 Å ³	$R_{\rm w}$ =5.11 χ^2 =1.89
	Orthorhombic	Pnma (89.85%)	<i>a</i> =5.5342(4)Å <i>b</i> =7.8068(7) Å <i>c</i> =13.5355(4)Å Volume=584.80Å ³	

Table S1. Details of Rietveld refinement structural parameters of the $Bi_{1-x}Sm_xFeO_3$ thin films based on the measured XRD data.



Fig. S1. Refinement results of $Bi_{1-x}Sm_xFeO_3$ thin films (a) x=0; (b) x=0.05; (c) x=0.10; (d) x=0.15.

References

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