

Supporting information

Morphology Control of BiFeO₃ Aggregates via Hydrothermal Synthesis

Authors

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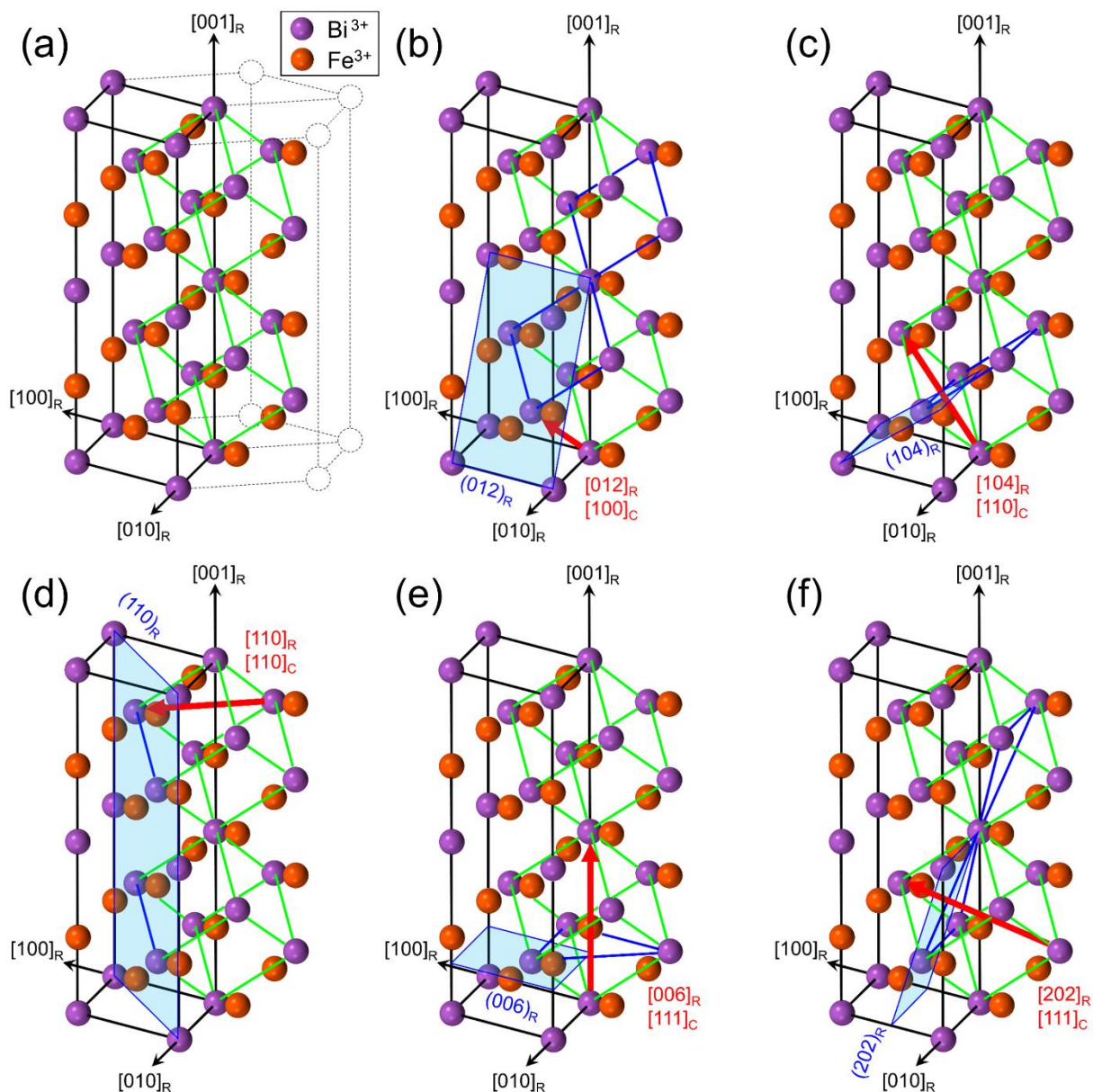
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(g)

$$\begin{pmatrix} h \\ k \\ l \end{pmatrix}_{\text{P-C}} = \begin{pmatrix} 1/3 & 2/3 & 1/6 \\ -2/3 & -1/3 & 1/6 \\ 1/3 & -1/3 & 1/6 \end{pmatrix} \begin{pmatrix} h \\ k \\ l \end{pmatrix}_{\text{R}}$$

(h)

Rhombohedral			Pseudo-Cubic		
<i>h</i>	<i>k</i>	<i>l</i>	<i>h</i>	<i>k</i>	<i>l</i>
0	1	2	1	0	0
1	0	4	1	1	0
1	1	0			
0	0	6	1	1	1
2	0	2			
0	2	4	2	0	0
1	1	6	2	1	0
1	2	2			
0	1	8	2	1	1
2	1	4			
3	0	0			

Figure S1 (a) Schematic of the BiFeO_3 unit cell in the hexagonal setting drawn with black lines with its axes, and pseudo-cubic setting drawn with green lines of $R3c$ space group. (b-f) Schematics of the correspondence faces between rhombohedral and cubic systems; a rhombohedral face shown by the light blue area in the R -unit, and the corresponding cubic face is drawn by the blue lines in the C -units. (g) Conversion matrix from rhombohedral $R3c$ to pseudo-cubic $Pm\bar{3}m$. After the conversion, the equivalent planes in the cubic system are required to unify, shown as $\{hkl\}$ ($h \geq k \geq l \geq 0$). (c) Table of the correspondence crystal faces between the rhombohedral $R3c$ and the pseudo-cubic $Pm\bar{3}m$ of space group in BiFeO_3 unit cell.

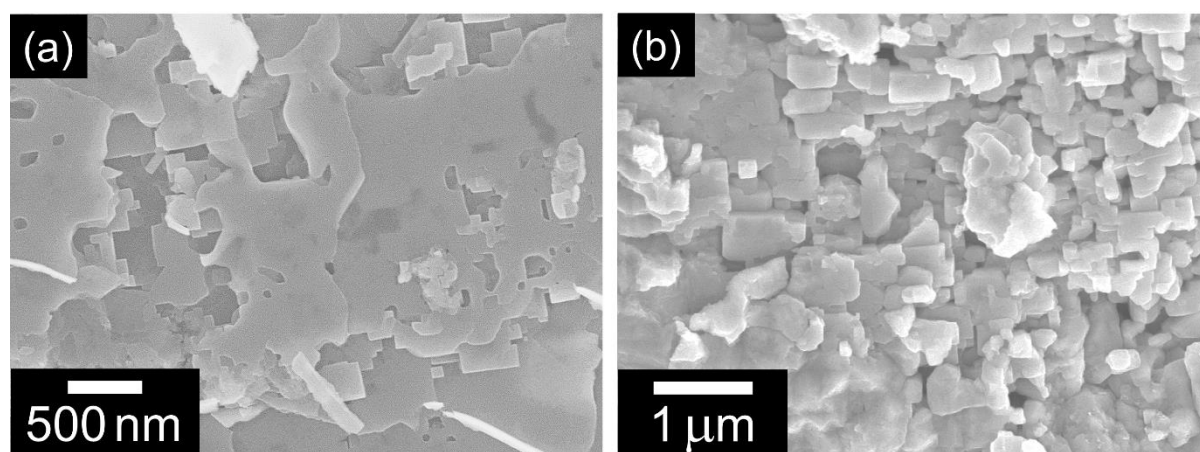


Figure S2 Magnified cross-sectional SEM images of the fractured surface of the BiFeO_3 aggregates prepared at (a) 10.00 and (b) 11.75 M KOH concentrations.

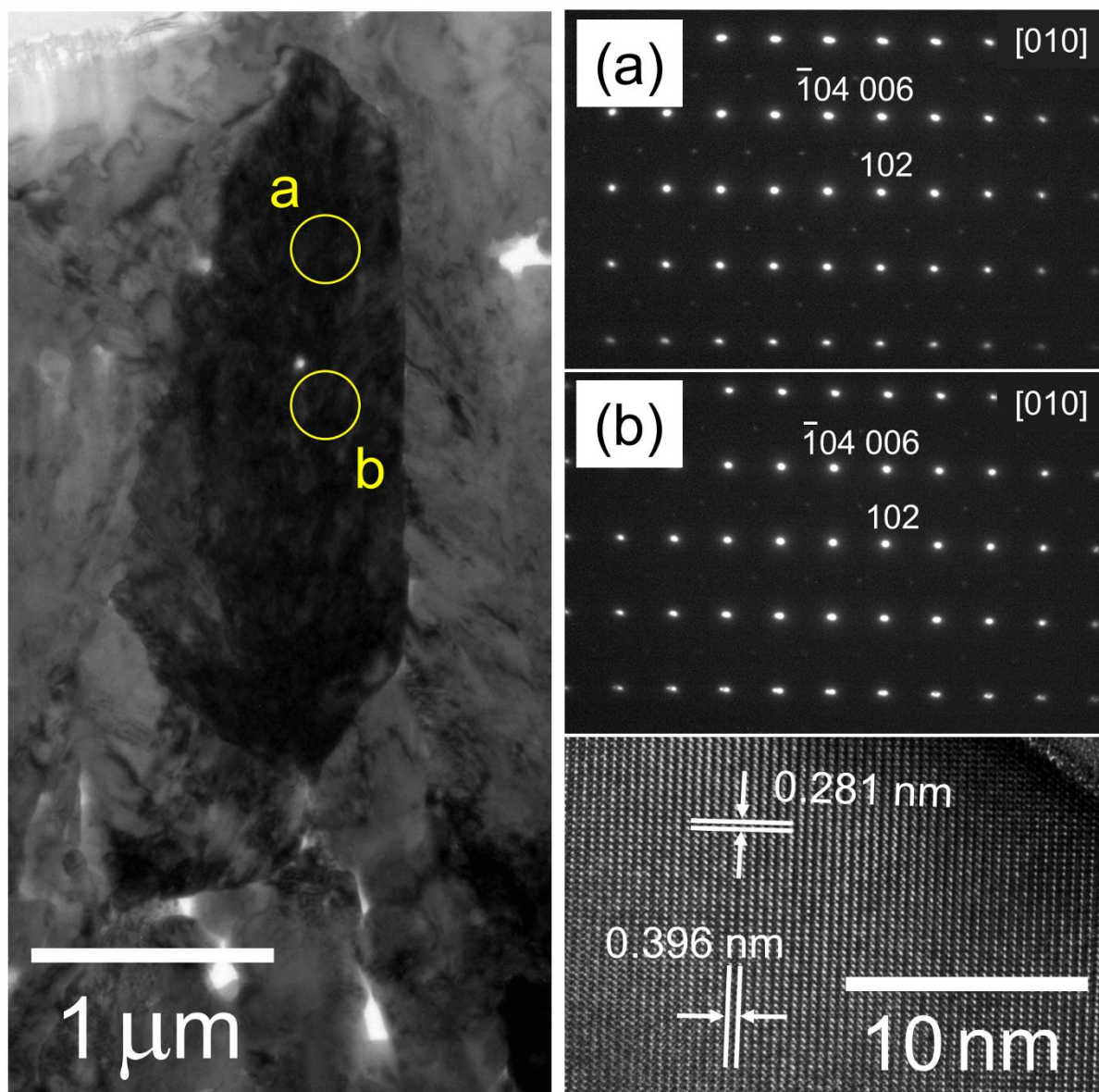


Figure S3 TEM images of a diffracted boat-shaped single-crystal (left image), with selected area electron diffraction (SAED) patterns taken from (a) and (b) points in the crystal (two upper right images). The SAED patterns at (a) and (b) were the same, and both are consistent with a rhombohedral phase BiFeO_3 $R3c$ structure. With regard to the weak spot located at (003) plane, it is considered an appearance of superlattice reflection. A high resolution (HR)-TEM of the diffracting crystal is shown in the bottom right image. The regular spacing of the observed lattice by HR-TEM are 0.396 and 0.281 nm, which are consistent with the (102) and (104) planes of the rhombohedral phase BiFeO_3 , respectively.

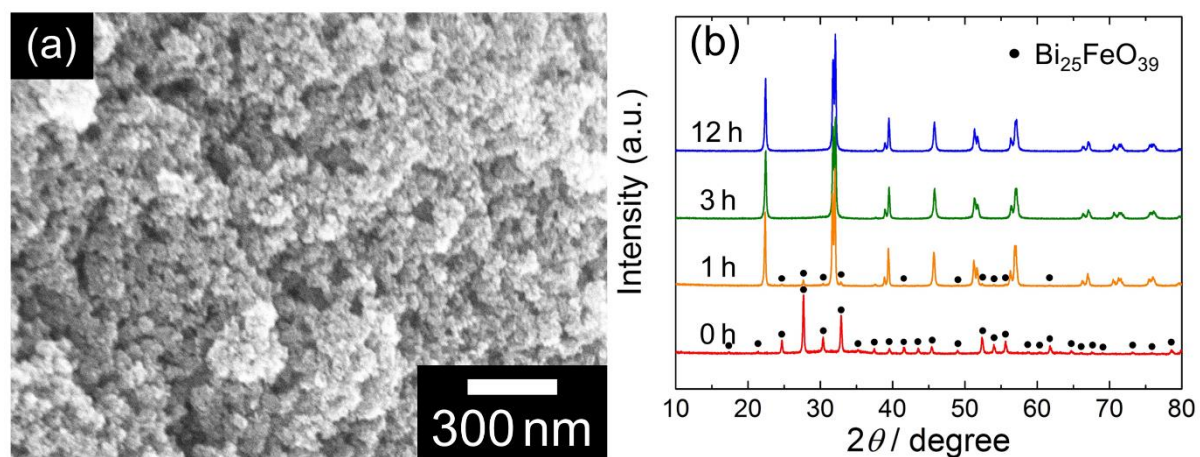


Figure S4 (a) SEM image of a sample prepared by hydrothermal reaction. The temperature was increased at a rate of $1^{\circ}\text{C}/\text{min}$ up to 200°C and hereupon the autoclave was allow to cool naturally to the room temperature (equivalent to the 0 h sample in (b)). (b) XRPD patterns of a sample as a function of hydrothermal reaction time. The temperature was increased at a rate of $1^{\circ}\text{C}/\text{min}$ from room temperature up to 200°C and was kept for various time periods (0–12 h).

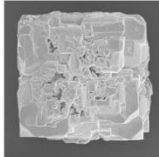
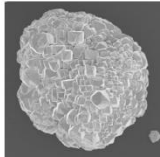
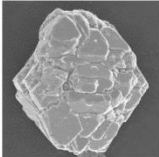
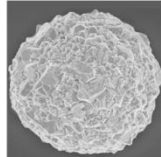
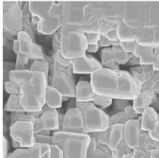
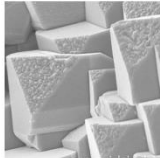
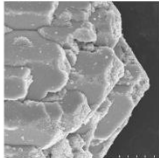
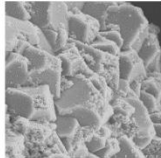
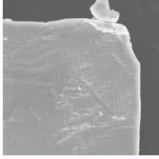
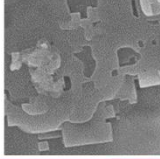
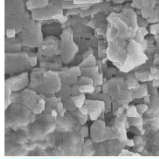
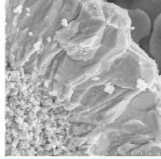
	KOH concentration (supersaturation)			
	← Low			High →
Morphology of aggregate				
	Cube		Octahedron	Sphere
Morphology of building units				
	Cubes	Truncated Cubes	Truncated Octahedra	
Aggregation between building units	Oriented Attachment			Random
Internal structure of aggregate				
	Dense		Sparse	

Figure S5 Schematic model of morphological evolution depending upon KOH concentration.