Supporting Information for

Oxygen release/incorporation behavior in hexagonal perovskite $BaFeO_3$ explored by $^{18}O/^{16}O$ isotope exchange reactions

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This supporting information consists of results of (1) Rietveld refinement for the 12R-type $BaFeO_3$ synthesized under a high-pressure condition, (2) Rietveld refinement for the 12R-type $BaFeO_3$ at room temperature after heating at 700 °C, and (3) *in situ* SXRD for the 12R-type $BaFeO_3$ in air at room temperature, 700 °C, and room temperature again.

(1) Results of Rietveld refinement for the 12R-type $BaFeO_3$ synthesized under a high-pressure condition are presented below.

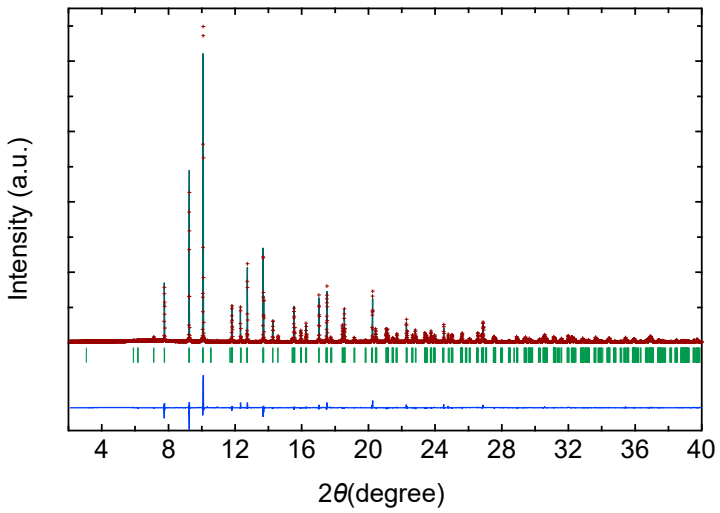

Fig. S1 SXRD pattern and Rietveld refinement result for the 12R-type $BaFeO_3$ at room temperature in air. The sample was synthesized under high-pressure condition. The diffraction data was collected with 0.500322 Å synchrotron X-ray at BL02B2 in SPring-8. The red plus marks and light blue lines represent the observed data and fitting patterns, respectively. The bottom blue lines represent the difference between observed and calculated intensities. The green vertical marks indicate the Bragg peak positions of the 12R-type structure.

Table S1 Crystallographic parameters refined from the SXRD data for the 12R-type $BaFeO_3$ at room temperature.

Space group *C*2/*m*, a = 9.85699(3) Å, b = 5.69807(2) Å, c = 9.89532(3) Å, and β = 109.5224(3). R_{wp} = 7.53% and R_p = 5.78%. All sites are fully occupied.

Atom	Site	x	y	z	B (Å^2)
Ba1	4*i*	0.2871(1)	0	0.8611(1)	0.48(2)
Ba2	4*i*	0.1262(1)	0	0.3806(1)	0.50(1)
Fe1	2*a*	0	0	0	0.57(5)
Fe2	2*d*	0	0.5	0.5	0.21(4)
Fe3	4*i*	0.4064(3)	0	0.2206(2)	0.39(4)
O1	4*i*	0.608(1)	0	0.374(1)	1.2(3)
O2	8*j*	0.382(1)	0.222(2)	0.374(1)	0.6(1)
O3	4*i*	0.204(2)	0	0.129(1)	1.1(3)
O4	8*j*	0.452(1)	0.246(2)	0.121(1)	0.5(1)

(2) Results of Rietveld refinement for the 12R-type $BaFeO_3$ at room temperature after heating at 700 °C are presented below.

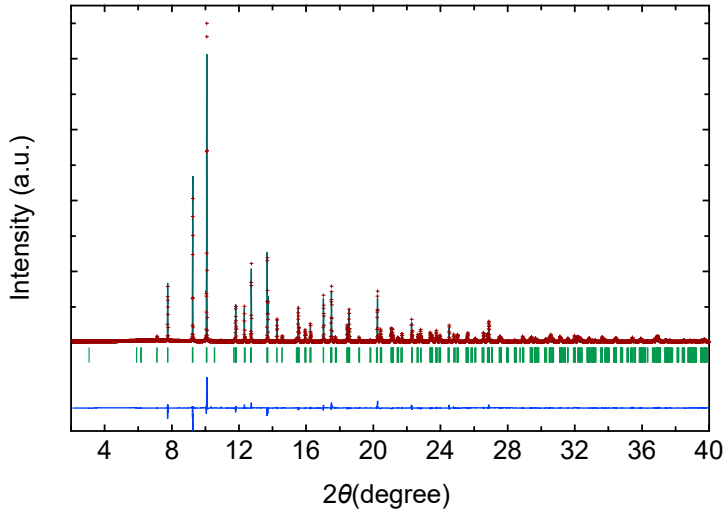

Fig. S2 SXRD pattern and Rietveld refinement result for the 12R-type $BaFeO_3$ at room temperature. The sample was annealed at 700 °C. The diffraction data was collected with 0.500322 Å synchrotron X-ray at BL02B2 in SPring-8. The red plus marks and light blue lines represent the observed data and fitting patterns, respectively. The bottom blue lines represent the difference between observed and calculated intensities. The green vertical marks indicate the Bragg peak positions of the 12R-type structure.

Table S2 Crystallographic parameters refined from the SXRD data for the 12R-type $BaFeO_3$ at room temperature after heating at 700 °C.

Space group *C*2/*m*, a = 9.85701(4) Å, b = 5.69782(2) Å, c = 9.89552(4) Å, and β = 109.5192(3). R_{wp} = 7.83% and R_p = 6.01%. All sites are fully occupied.

Atom	Site	x	y	z	B (Å^2)
Ba1	4*i*	0.2867(1)	0	0.8611(1)	0.52(2)
Ba2	4*i*	0.1262(1)	0	0.3804(1)	0.42(2)
Fe1	2*a*	0	0	0	0.38(5)
Fe2	2*d*	0	0.5	0.5	0.20(4)
Fe3	4*i*	0.4060(3)	0	0.2197(2)	0.50(4)
O1	4*i*	0.610(1)	0	0.375(1)	0.8(3)
O2	8*j*	0.381(1)	0.222(2)	0.374(1)	0.7(2)
O3	4*i*	0.201(2)	0	0.130(1)	1.1(3)
O4	8*j*	0.451(1)	0.239(2)	0.120(1)	0.6(1)

(3) Results of *in situ* SXRD for the 12R-type $BaFeO_3$ in air at room temperature, 700 °C, and room temperature again are presented below.

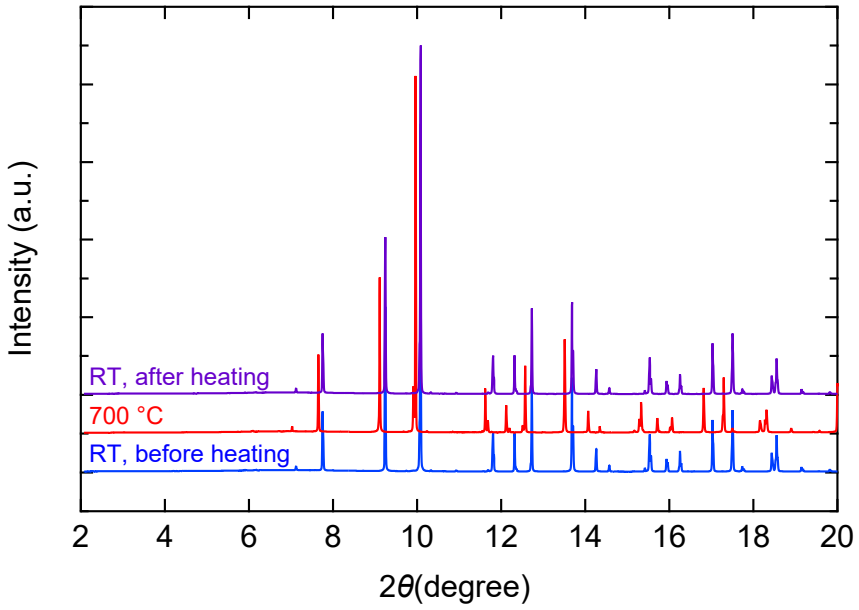

Fig. S3 SXRD diffraction patterns for the 12R-type $BaFeO_3$ in air at room temperature, 700 °C, and room temperature again.