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Supplementary Information

Improved oxide-ion conductivity of $NdBaInO_4$ by Sr doping

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A) Rietveld patterns for synchrotron X-ray powder diffraction data (BL19B2 beam line of SPring-8) of $Nd_{0.9}Sr_{0.1}BaInO_{3.95}$

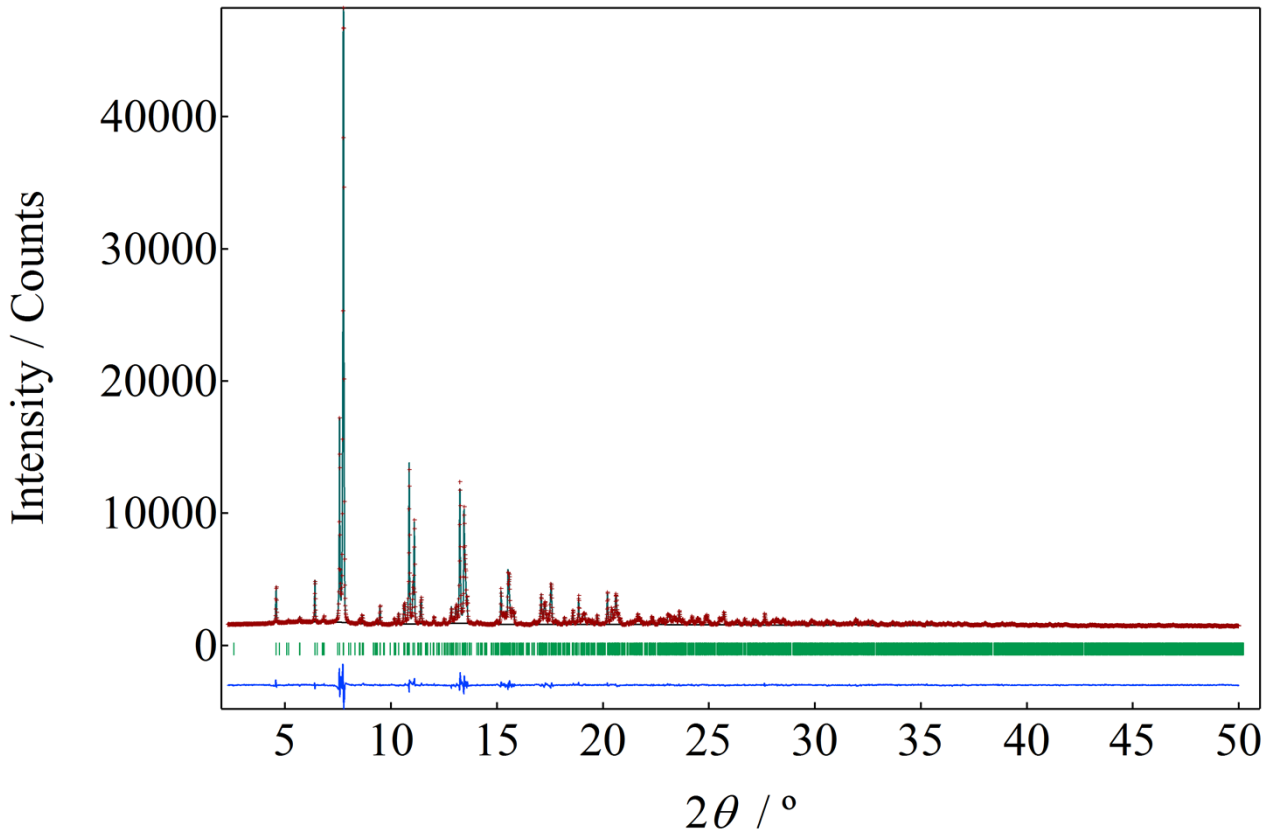

Figure S3. Rietveld pattern for synchrotron X-ray powder diffraction (XRPD) data of $Nd_{0.9}Sr_{0.1}BaInO_{3.95}$ taken at 27 °C showing the experimental (red + marks), calculated (green solid line) and difference (blue lower lines) plots. Green tick marks indicate Bragg peak positions. Synchrotron XRPD measurements were carried out by the Debye-Scherrer camera installed at the beam line BL19B2 of SPring-8 (wavelength = 0.399662(2) Å).

B) Crystallographic data of $Nd_{0.9}Sr_{0.1}BaInO_{3.95}$

Table S1. Crystallographic data of $Nd_{0.9}Sr_{0.1}BaInO_{3.95}$.

Atomic coordinates and atomic displacement parameters of $Nd_{0.9}Sr_{0.1}BaInO_{3.95}$ obtained from the synchrotron X-ray powder diffraction data (BL19B2, SPring-8) measured at 27 °C						
Label	site	*g*	*x*	*y*	*z*	*U* (Å^2)
Nd	4*e*	0.9	0.45225(15)	0.7522(17)	0.1066(3)	0.0048(5)
Sr	4*e*	0.1	0.45225 (= x_{Nd})	0.7522 (= y_{Nd})	0.1066 (= z_{Nd})	0.0048 (= U_{Nd})
Ba	4*e*	1	0.14846(18)	0.2476(15)	0.0339(4)	0.0100(5)
In	4*e*	1	0.8318(2)	0.249(3)	0.2050(4)	0.0031(4)
O1	4*e*	0.9875	0.1782(16)	0.797(2)	0.043(4)	0.0200 (= 2×U_{Ba})**
O2	4*e*	0.9875	−0.006(5)	0.022(7)	0.266(5)	0.0200 (= 2×U_{Ba})
O3	4*e*	0.9875	0.373(3)	0.500(4)	0.323(4)	0.0200 (= 2×U_{Ba})
O4	4*e*	0.9875	0.643(3)	0.454(4)	0.126(3)	0.0200 (= 2×U_{Ba})

* x_{Nd} , y_{Nd} and z_{Nd} stand for the atomic coordinates of Nd atom.

** U_X denotes the isotropic atomic displacement parameter of *X* atom.

Atomic coordinates and displacement parameters of $Nd_{0.9}Sr_{0.1}BaInO_{3.95}$ obtained from the angle dispersive type neutron powder diffraction data (HRPD, HANARO) measured at 800 °C						
Label	site	*g*	*x*	*y*	*z*	*U* (Å^2)
Nd	4*e*	0.9	0.4524(2)	0.7518 (19)	0.1152 (15)	0.0357 (9)
Sr	4*e*	0.1	0.4524(= x_{Nd})	0.7518 (= y_{Nd})	0.1152 (= z_{Nd})	0.0357 (= U_{Nd})
Ba	4*e*	1	0.1477(4)	0.253(3)	0.031(2)	0.0458(13)
In	4*e*	1	0.8311(5)	0.242(2)	0.203(2)	0.0328(14)
O1	4*e*	0.975	0.1829(4)	0.758(4)	0.042(2)	0.0623 (U_{eq})**
O2	4*e*	0.975	0.0021(16)	0.011(2)	0.2613(15)	0.0532(15)
O3	4*e*	0.975	0.3746(10)	0.521(2)	0.341(2)	0.066(3)
O4	4*e*	0.975	0.6410(10)	0.491(2)	0.152(2)	0.0702 (U_{eq})

***	U_{11} (Å^2)	U_{22} (Å^2)	U_{33} (Å^2)	U_{12} (Å^2)	U_{13} (Å^2)	U_{23} (Å^2)
O1	0.00039(2)	0.00117(4)	0.00037(4)	0.00009(8)	0.00019(8)	−0.00016(8)
O4	0.00048(4)	0.00057(4)	0.00090(7)	0.00033(3)	−0.00017(7)	0.00034(8)

** Equivalent isotropic atomic displacement parameter. *** U_{ij}: Anisotropic atomic displacement parameter.

C) The site preference of Sr in the $Nd_{0.9}Sr_{0.1}BaInO_{3.95}$

In the preliminary analysis, the site preference of Sr in $Nd_{0.9}Sr_{0.1}BaInO_{3.95}$ was investigated. There are three sites for the cations (Nd, Ba and In). The refinements based on the time-of-flight neutron diffraction data were carried out using three structure models as shown in Table S2. The model 1 in which the Sr exists at the Nd site gave the best *R*-factors.

Table S2. Results of the refinements for the three structure models of $Nd_{0.9}Sr_{0.1}BaInO_{3.95}$

Site name	Model 1	Model 2	Model 3
Nd	g(Nd) = 0.9, g(Sr) = 0.1	g(Nd) = 0.9, g(Ba) = 0.1	g(Nd) = 0.9, g(In) = 0.1
Ba	g(Ba) = 1	g(Ba) = 0.9, g(Sr) = 0.1	g(Ba) = 1
In	g(In) = 1	g(In) = 1	g(In) = 0.9, g(Sr) = 0.1
R factors			
R_{wp}	0.0458	0.0459	0.0462
R_B	0.0534	0.0567	0.0572

D) Definition of the average thermal expansion coefficients

In this paper, the average thermal expansion coefficients between T_{min} and T_{max} (°C) are defined as follow. Here x is the unit cell parameter a, b, c or β and V is the unit cell volume.

$$\alpha_x = \frac{x_{T_{max}} - x_{T_{min}}}{x_{T_{min}} \times (T_{max} - T_{min})}$$

$$\bar{\alpha} = \frac{V_{T_{max}}^{\frac{1}{3}} - V_{T_{min}}^{\frac{1}{3}}}{V_{T_{min}}^{\frac{1}{3}} \times (T_{max} - T_{min})}$$

E) Thermogravimetric analysis and differential thermal analysis

Thermogravimetric analyses (TGA) of $NdBaInO_4$ and $Nd_{0.9}Sr_{0.1}BaInO_{3.95}$ in Ar flow (50 mL min^{-1}) were carried out using a Bruker-AXS TG-DTA2020SA instrument at the heating and cooling rates of 10 °C min^{-1}. The TG measurements were repeated three times to confirm the reproducibility and to prevent from the influence of the absorbed species such as water. The result is shown in Figure S4.

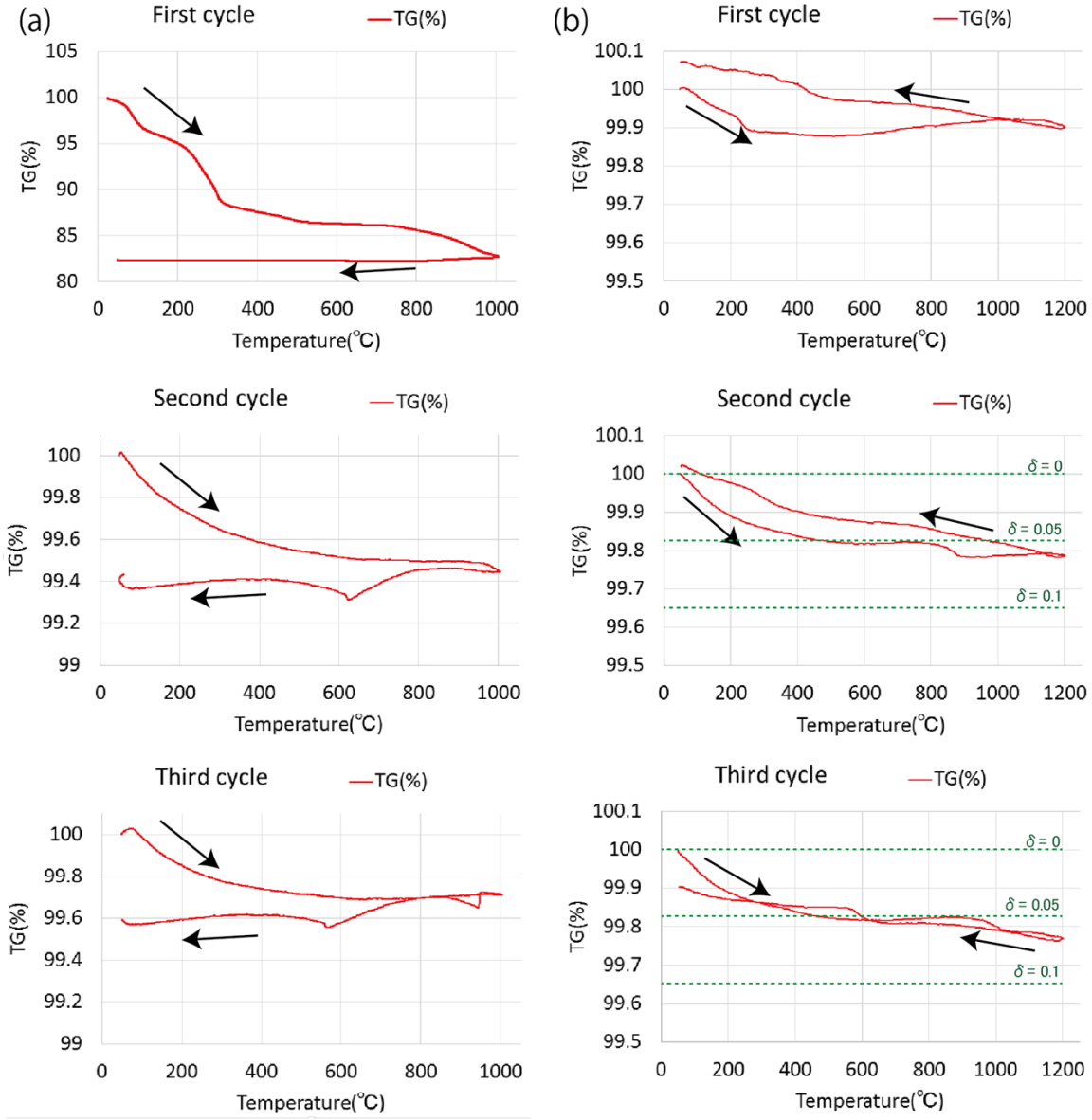

Figure S4. Results of the thermogravimetric analysis (TGA; red lines) of (a) $NdBaInO_4$ and (b) $Nd_{0.9}Sr_{0.1}BaInO_{3.95}$. The green dash lines indicate the δ of $Nd_{0.9}Sr_{0.1}BaInO_{3.95-\delta}$.

End of the Supporting Information.