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Effects of flux treatment on morphology of single-crystalline $BaNbO_2N$ particles

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Electronic Supplementary information

Contents

(1) XRD patterns for $BaNbO_2N$ treated using different alkali chloride fluxes

Figure S1 shows magnified regions of the XRD patterns in Figure 1 in the 2θ range of 30–60°. For $BaNbO_2N$(NaCl), $BaNbO_2N$(KCl) and $BaNbO_2N$(RbCl), diffraction peaks associated with NbO_xN_y phases were also observed, indicating the chemical reduction of Nb species during the flux treatment. Figure S2 shows the 2θ range of 63–64.4°. Splitting of the (220) peak can be observed, corresponding to $K_{\alpha 1}$ and $K_{\alpha 2}$. After the flux treatment, the splitting became more pronounced, indicating an improvement in crystallinity. The dashed line indicates the (220) peak position for $BaNbO_2N$ before treatment. For $BaNbO_2N$(NaCl) and $BaNbO_2N$(CsCl), the split peak shifted to higher and lower angles, respectively.

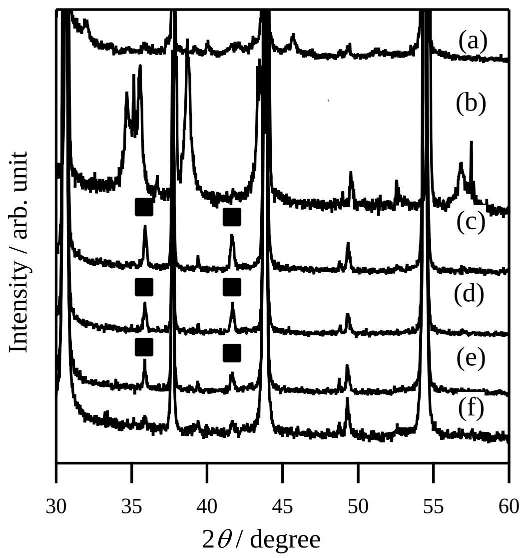

Figure S1. XRD patterns for $BaNbO_2N$ particles (a) before and after flux treatment with (b) LiCl, (c) NaCl, (d) KCl, (e) RbCl, and (f) CsCl. Square symbols (■) indicate NbO_xN_y.

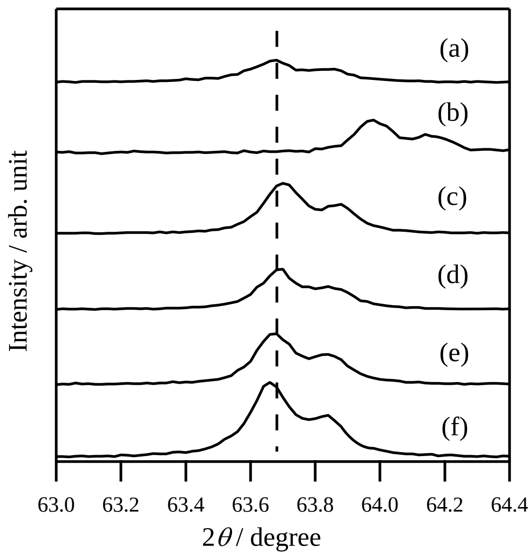

Figure S2. XRD patterns for $BaNbO_2N$ particls (a) before and after flux treatment with (b) LiCl, (c) NaCl, (d) KCl, (e) RbCl, and (f) CsCl.

(2) Schematic illustration of two-boat flux treatment setup

Figure S3 shows a schematic illustration of the two-boat flux treatment setup. Two alumina boats were inserted inside an alumina tube and were heated under an NH_3 flow. An NaCl flux and $BaNbO_2N$ particles was placed in the upstream and downstream boats, respectively. During the flux treatment, both boats were heated to the same temperature.

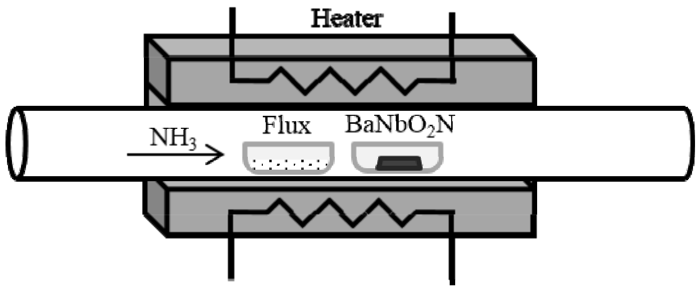

Figure S3. Schematic illustration of two-boat flux treatment setup.

(3) Elemental analysis

Elemental analysis results for $BaNbO_2N$ before and after flux treatment with NaCl, KCl, RbCl, and CsCl are shown in Table S1. The amount of Ba, Nb, and alkali metal (except Cs) was determined by ICP-AES. The amount of Cs was determined by XRF. The amount of O and N was determined by combustion analysis.

Table S1. Elemental analysis results (atomic ratio) before and after flux treatment using alkali chlorides.

Flux	Cation of flux	Ba[a]	Nb[a]	O[b]	N[b]
–	–	1.00	0.91	2.66	0.80
NaCl	0.05[a]	1.00	1.11	2.24	1.11
KCl	0.02[a]	1.00	1.04	2.03	1.03
RbCl	0.005[a]	1.00	1.04	2.02	1.05
CsCl	0.03[c]	1.00	1.02	2.07	1.00

[a] Determined by ICP analysis
[b] Determined by combustion analysis
[c] Determined by XRF analysis