

Supporting Information for

Silicone-oil-assisted synthesis of high-quality sodium niobate nanowires

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Experimental Procedure

Chemicals

Niobium oxide (Alfa Aesar, 99.9985%), sodium hydroxide (Alfa Aesar, 98%), silicone oil (Dow Corning, viscosity: 100 cs), and anhydrous ethanol (99.7%) were purchased and used without further purification.

Synthesis of Na₂Nb₂O₆·H₂O Nanowires

Nanowires of Na₂Nb₂O₆·H₂O were synthesized by a silicone-oil-assisted hydrothermal method. In a typical process, 0.75 mmol Nb₂O₅ (0.2 g) was added into the NaOH solution (30 ml, 10 M), followed by the addition of silicone oil under continuous stirring. After magnetic stirring for 2 hours, the obtained transparent solution was transferred into a 50 mL Teflon-lined stainless steel autoclave to undergo hydrothermal reaction at 150 °C for 5 hours in an oil bath under magnetic stirring. After cooled down to room temperature, the obtained white precipitate was washed with deionized water and ethanol for several times, and dried at 80 °C. To investigate the effect of silicone oil on the synthesis of Na₂Nb₂O₆·H₂O nanowires, different amount of silicone oil (0 ml, 0.1 ml, 0.25 ml, 0.5 ml, 1 ml, 2 ml) were used in this process.

Synthesis of Na₂Nb₂O₆·H₂O Nanowires

NaNbO₃ nanowires were obtained through phase transformation of Na₂Nb₂O₆·H₂O by annealing treatment at 500 °C for 4 hours.

Characterization

The crystal structure and phase composition were characterized by X-ray diffraction (XRD) (Rint-2000V/PC diffractometer, Rigaku, Japan) with Cu/K α radiation ($\lambda = 1.5406 \text{ \AA}$). The microstructure of the products was imaged using scanning electron microscopy (SEM, S4800, Zeiss, Japan, 5 KV) and transmission electron microscopy (TEM, Tecnai G2 F30, FEI, USA, 300 KV). Dehydration process and temperature of phase transition of products were analyzed by Thermogravimetric analysis and differential

scanning calorimetry (TGA/DSC, STA 449 F3, N₂ flow ~ 10 ml·min⁻¹, heating rate ~ 10 K·min⁻¹). Fourier Transform infrared spectroscopy (FTIR) was conducted with Thermo Scientific Nicolet iS 50.

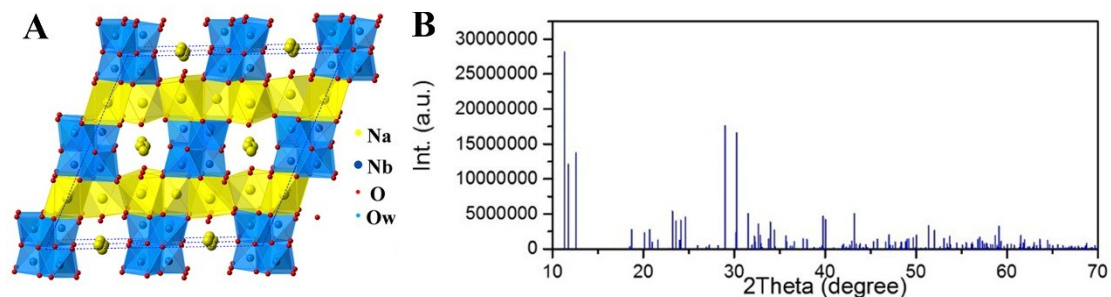


Figure S1. (A) Crystal structure of Na₂Nb₂O₆·H₂O nanowire, and the yellow, blue, red and cyan spheres represent Na, Nb, O and Ow atoms, respectively (Ow represents O of H₂O molecules); (B) the according XRD pattern obtained by using crystals impact diamond 3¹.

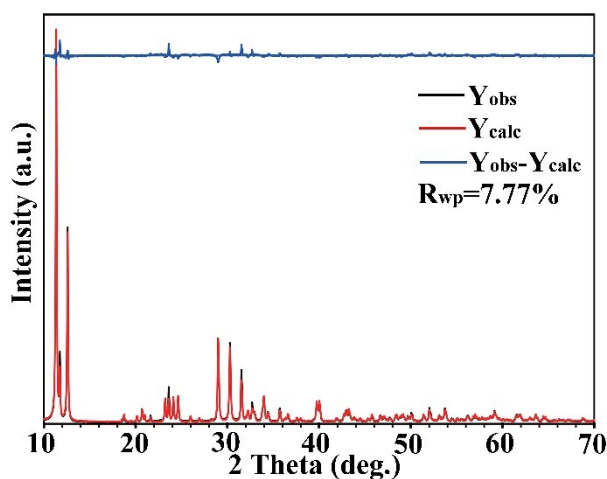


Figure S2. The observed (black), calculated (red) and difference (blue) profile of Na₂Nb₂O₆·H₂O nanowires.

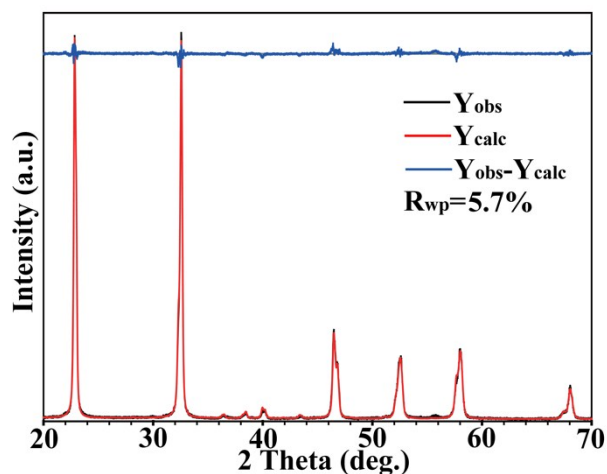
Table S1. Refined cell parameters of as-prepared Na₂Nb₂O₆·H₂O phase (Space Group C2/c) in comparison with standard data.

Cell parameters	a (Å)	b(Å)	c(Å)	α(°)	β(°)	γ(°)
Refined	17.0503	5.0272	16.4850	90.0	113.9394	90.0
Standard*	17.0511	5.0293	16.4921	90.0	113.9420	90.0

*: Obtained from Crystallography Open Database (COD).

Table S2. Atomic Coordinates of as-prepared $\text{Na}_2\text{Nb}_2\text{O}_6 \cdot \text{H}_2\text{O}$ phase.

atom	x	y	z
Na1	0.335	-0.366	0.734
Na2	0.5	0.14	0.75
Na3	0.263	0.288	0.012
Nb1	0.405	0.046	0.906
Nb2	0.533	0.549	0.915
O1	0.461	-0.254	-0.004
O2	0.477	-0.148	0.849
O3	0.42	0.359	0.85
O4	0.378	0.249	0.993
O5	0.6	0.418	0.861
O6	0.302	-0.094	0.837
O7	0.199	0.505	0.869

**Figure S3.** The observed (black), calculated (red) and difference (blue) profile of NaNbO_3 nanowires.**Table S3.** The refined cell parameters of as-prepared NaNbO_3 phase (Space group $P21ma$) in comparison with standard data.

Cell parameters	a(Å)	b(Å)	c(Å)	$\alpha(^{\circ})$	$\beta(^{\circ})$	$\gamma(^{\circ})$
Refined	5.5588	7.776	5.5105	90.0	90.0	90.0
Standard*	5.569	7.79	5.518	90.0	90.0	90.0

*: Obtained from COD.

Table S4. Atomic Coordinates of as-prepared NaNbO₃ phase.

atom	x	y	z
Na1	0.252	0.0	0.739
Na2	0.28	0.5	0.742
Nb1	0.27	0.251	0.244
O1	0.24	0.0	-0.31
O2	0.221	0.5	0.19
O3	0.026	0.28	0.539
O4	-0.046	0.021	0.038

Reference:

1. H. Xu, M. Nyman, T. M. Nenoff and A. Navrotsky, *Chemistry of materials*, 2004, **16**, 2034-2040.