

Supporting information

Black lithium niobate single crystal: influence of point defects on its microwave properties

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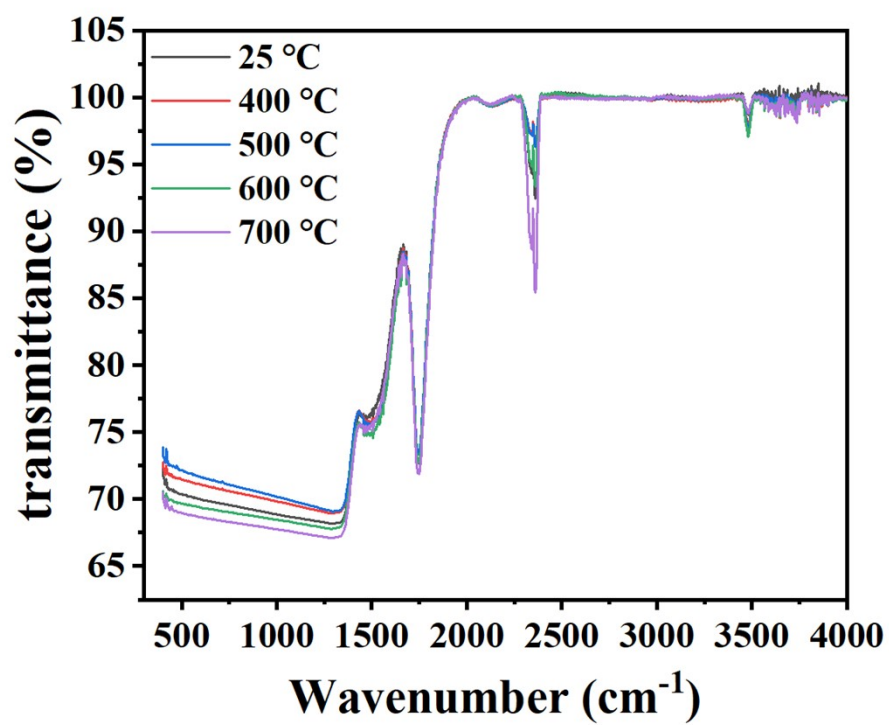


Fig. S1. Full spectrum of infrared transmittance of black lithium niobate wafers in the wavelength range of 300-4000 cm⁻¹

Table S1 The detailed characteristics of the three fitted peaks in the infrared (IR) absorption spectra of lithium niobate under untreated (25 °C) and different reduction temperature treatments (400 °C, 500 °C, 600 °C, and 700 °C)

Sample (°C)	Crest number	Crest area (cm ⁻²)	Percentage of crest area (%)	Peak position (cm ⁻¹)	Peak intensity (cm ⁻¹)	FWHM (cm ⁻¹)
25	A	2.88	22.4	3468.3	0.16	13.93
	B	7.26	56.5	3481.5	0.30	17.11
	C	2.70	21.0	3492.82	0.15	14.70
400	A	2.99	17.9	3467.5	0.26	11.48
	B	10.07	60.1	3480.2	0.49	16.25
	C	3.68	22.0	3491.2	0.25	15.28
500	A	3.74	18.2	3467.5	0.28	11.24
	B	10.90	53.0	3479.6	0.49	16.16
	C	5.93	28.8	3489.7	0.29	16.59
600	A	3.83	16.9	3467.4	0.32	10.67
	B	10.96	48.3	3479.3	0.54	15.64
	C	7.92	34.9	3489.3	0.37	18.38
700	A	1.44	15.6	3467.1	0.18	9.21
	B	5.44	58.6	3480.0	0.29	15.94
	C	2.40	25.8	3490.9	0.16	2.40

Table S2 Three fitting peak areas and O₂ concentration ratios of lithium niobate O 1s under untreated (25 °C) and different reduction temperature treatments (400 °C, 500 °C, 600 °C, and 700 °C)

Sample (°C)	Fitting the peak state	Fitting the peak area	O ₂ concentration ratio (%)
25	O ₁	255039.2	11.4
	O ₂	47817.68	
	O ₃	116777.37	
400	O ₁	377507.6	13.0
	O ₂	66958.73	
	O ₃	70784.16	
500	O ₁	182925.43	16.7
	O ₂	48928.91	
	O ₃	61193.73	
600	O ₁	187212.34	21.8
	O ₂	91714.45	
	O ₃	142267.3	
700	O ₁	229206.38	30.7
	O ₂	108511.11	
	O ₃	15432.57	

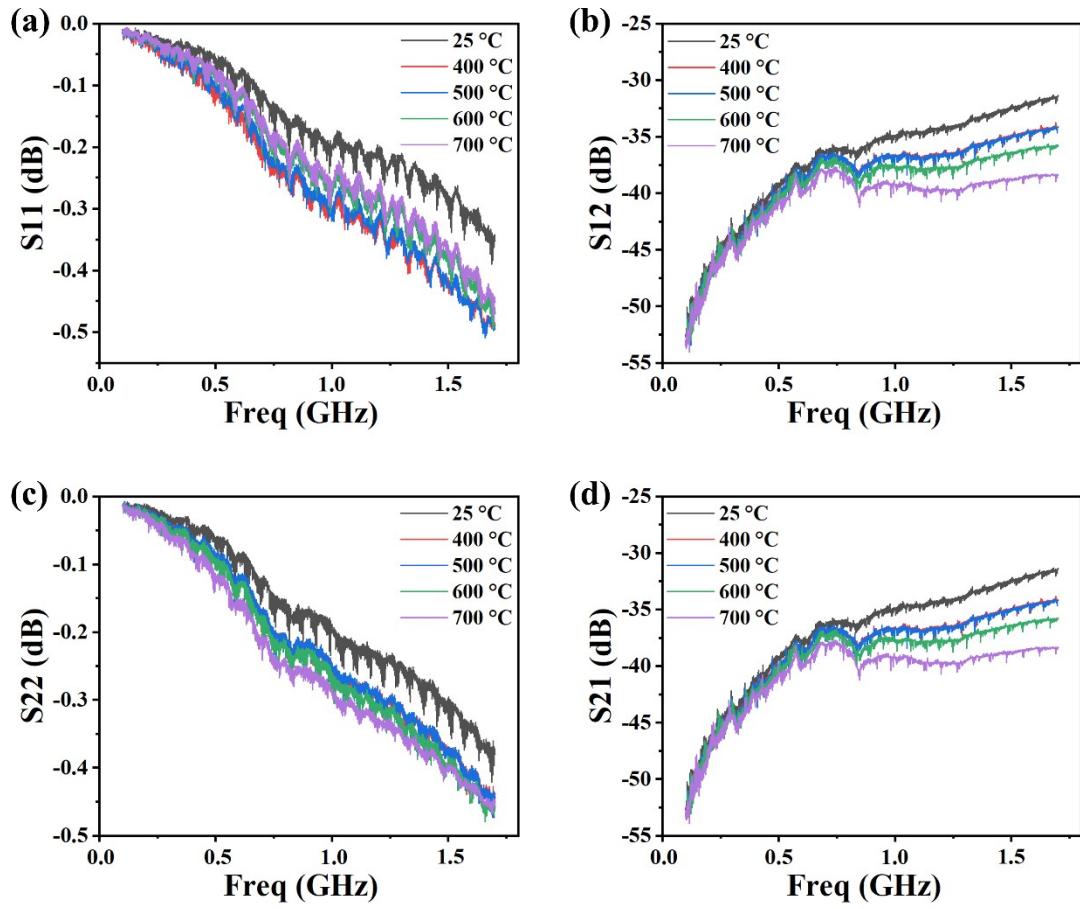


Fig. S2. S-parameters of lithium niobate under untreated (25 °C) and different reduction temperature treatments (400 °C, 500 °C, 600 °C, and 700 °C) in the frequency range of 0.1 GHz-1.7 GHz. (a) S11, (b) S12, (c) S22 and (d) S21.

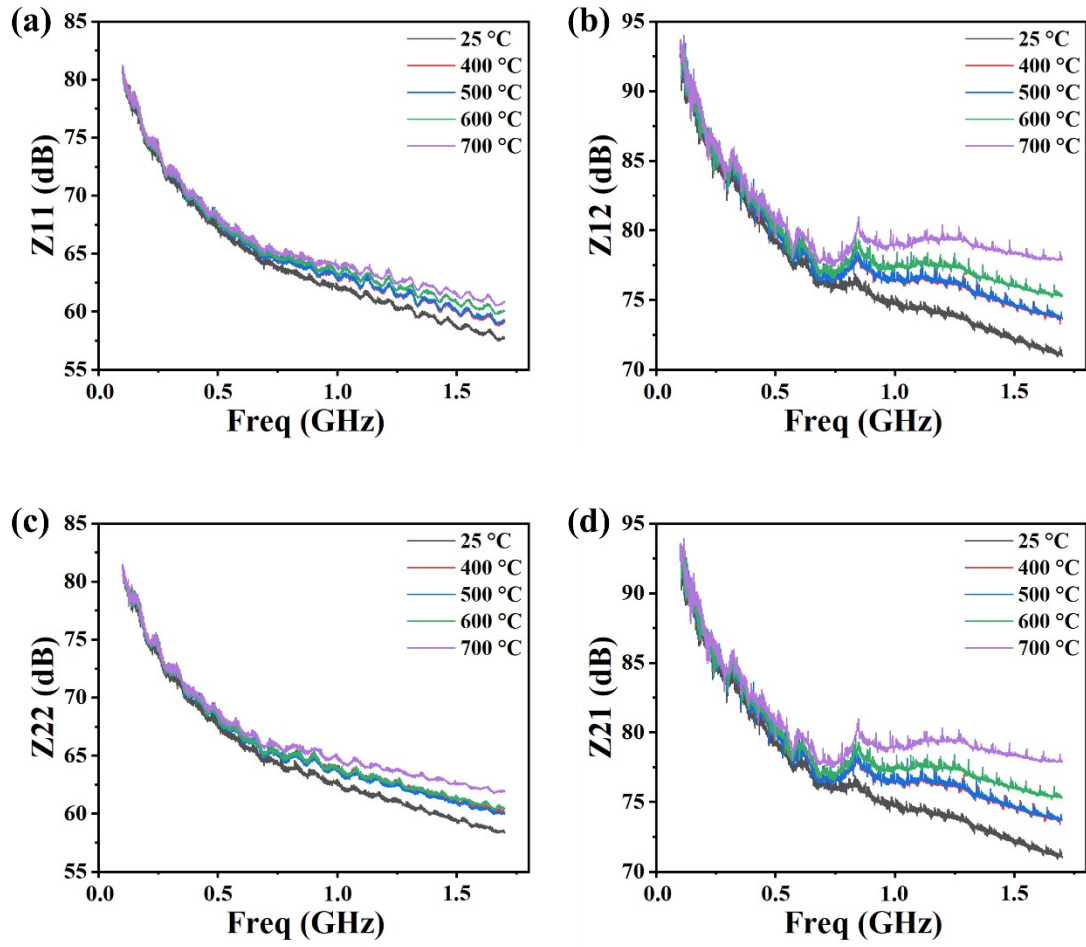


Fig. S3. Impedance values of lithium niobate under untreated (25 °C) and different reduction temperature treatments (400 °C, 500 °C, 600 °C, and 700 °C) in the frequency range of 0.1 GHz-1.7 GHz. (a) Z_{11} , (b) Z_{12} , (c) Z_{22} and (d) Z_{21} .

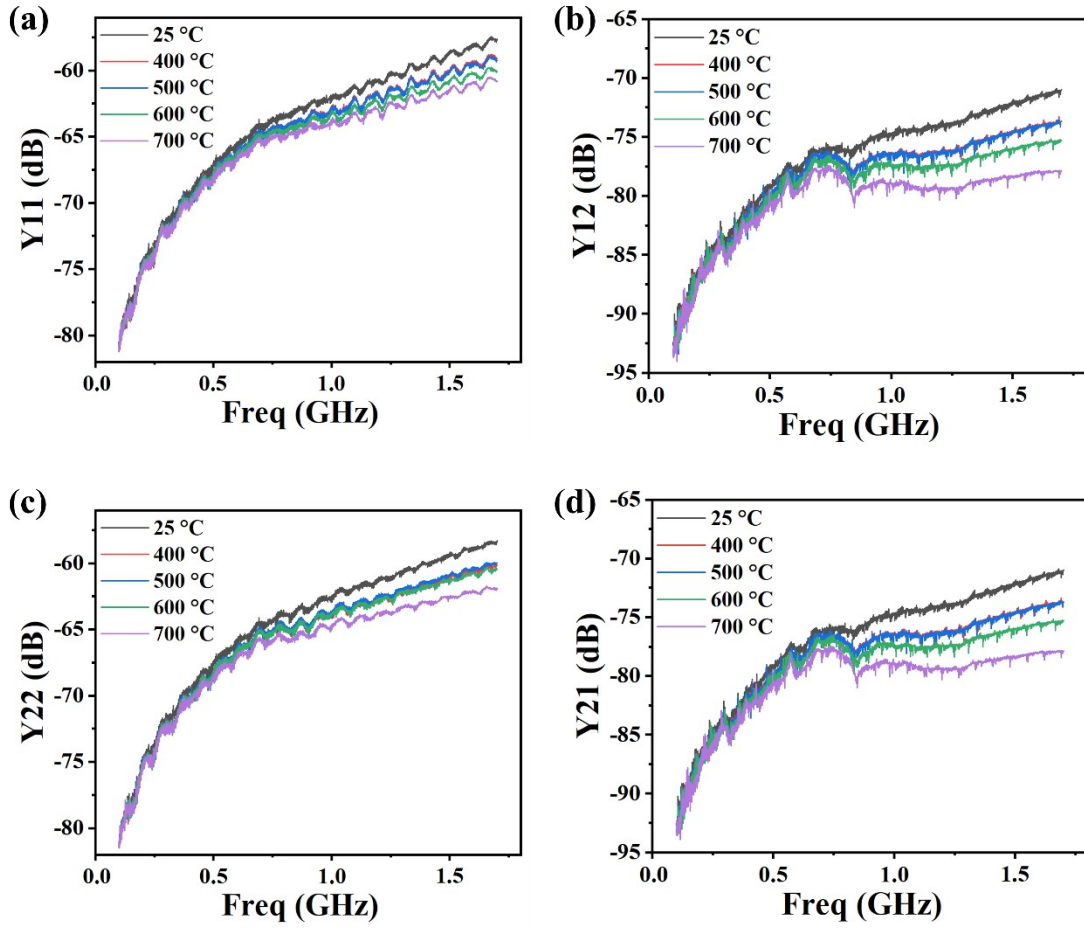


Fig. S4. The admittance of lithium niobate under untreated (25 °C) and different reduction temperature treatments (400 °C, 500 °C, 600 °C, and 700 °C) in the frequency range of 0.1 GHz-1.7 GHz. (a) Y11, (b) Y12, (c) Y22 and (d) Y21.

Table S3 The dielectric loss of lithium niobate under untreated (25 °C) and different reduction temperature treatments (400 °C, 500 °C, 600 °C, and 700 °C) at various frequency points (0.1 GHz, 0.5 GHz, 1.0 GHz, 1.5 GHz, and 1.7 GHz).

Sample (°C)	Frequency (GHz)	Substrate loss (dB)
25	0.1	0.0022
	0.5	0.0147
	1.0	0.0445
	1.5	0.0614
	1.7	0.0772
400	0.1	0.0026
	0.5	0.0199
	1.0	0.0569
	1.5	0.0790
	1.7	0.0984
500	0.1	0.0027
	0.5	0.0207
	1.0	0.0591
	1.5	0.0825
	1.7	0.1023
600	0.1	0.0026
	0.5	0.0243
	1.0	0.0672
	1.5	0.0915
	1.7	0.1076
700	0.1	0.0033
	0.5	0.0263
	1.0	0.0695
	1.5	0.0930
	1.7	0.1062