Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Supporting information

Microstructure and defect characters of lithium niobate with different Li concentrations

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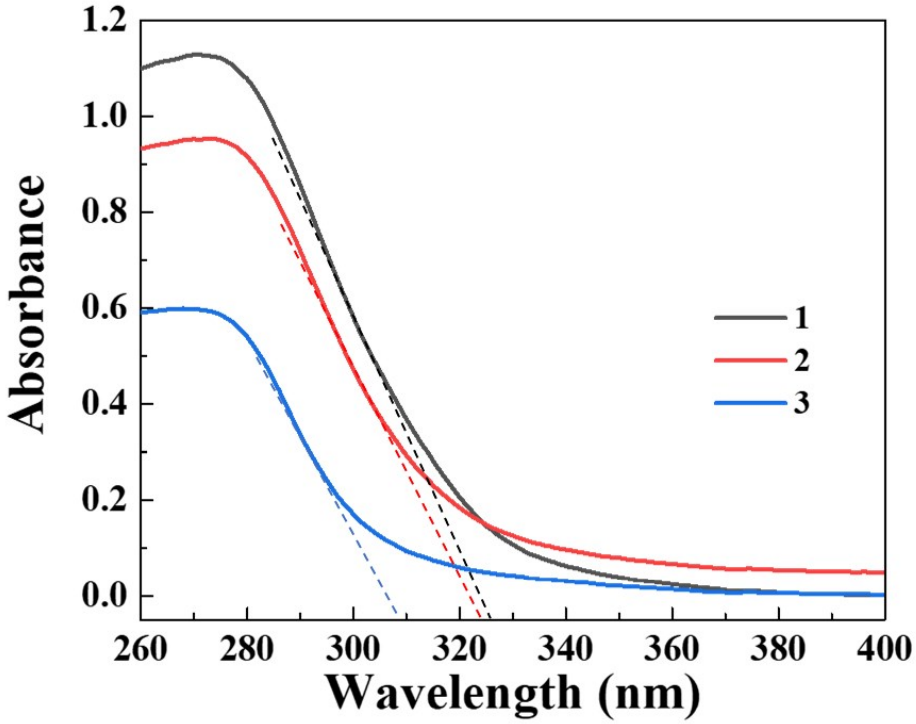


Fig. S1 UV-Vis absorption spectra of LN powder samples with different Li amounts.

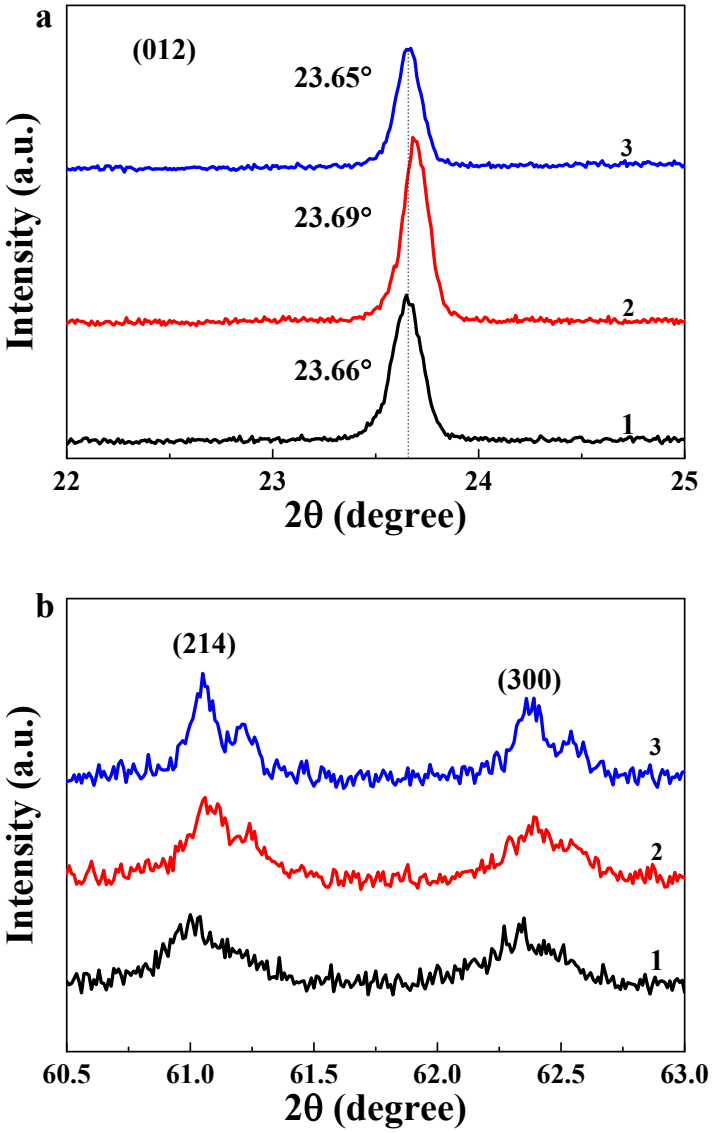


Fig. S2 Zoomed XRD patterns of the as-prepared LN samples with different Li amounts. (a) peak of (012) plane, (b) peaks of (214) and (300) planes.

Table S1 Frequencies of TO and LO phonons of symmetry A1 and E on congruent LN crystal.[1,2]

Modes	A_1(TO)/cm^{-1}	A_1(LO)/cm^{-1}	Motion
1	254	272	Nb z, O z
2	275	332	Nb z, Li z
3	332	419	O x y
4	631	871	O x y
Modes	E(TO)/cm^{-1}	E(LO)/cm^{-1}	Motion
1	152	186	Nb x, y, O x, y
2	186	194	(all)
3	236	238	(all)
4	263	295	(all)
5	322	366	(all)
6	369	425	(all)
7	432	456	(all)
8	578	625	(all)
9	738	880	Nb x y, O x y

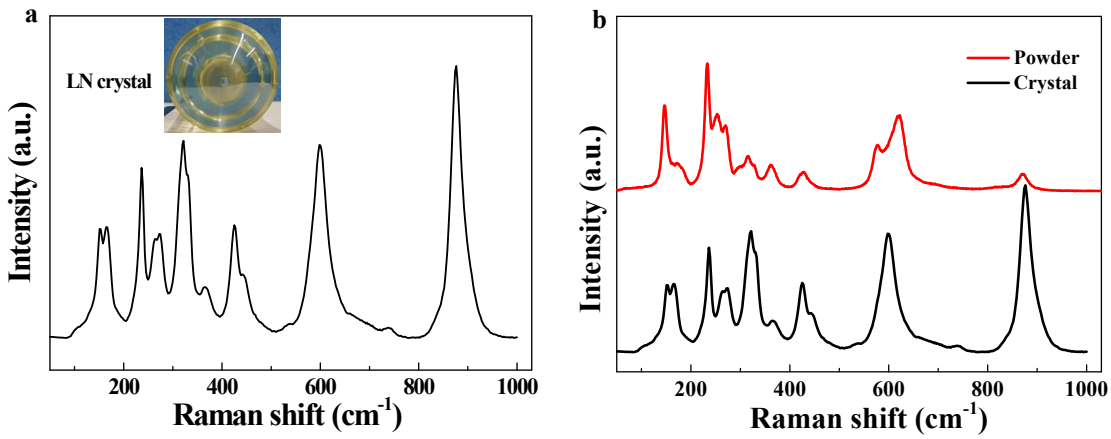
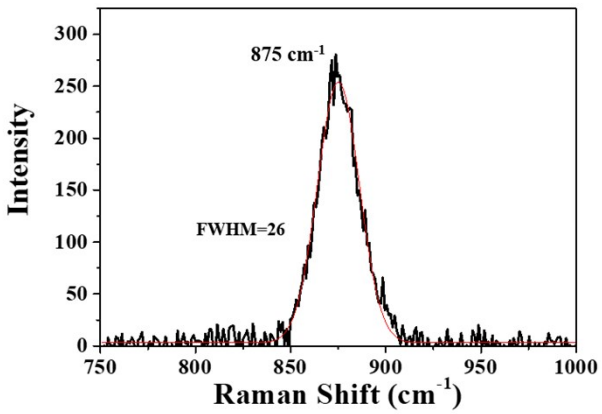


Fig. S3 Raman spectra of the as-grown LN single crystal (a) and 1# LN powder sample (b). Inset of (a) is photograph of LN single crystal along the *c*-direction grown by Czochralski method within our lab.



Model	Gauss		
Equation	y=y0+(A/(w*sqrt(PI/2)))*exp(-2*((x-xc)/w)^2)		
Reduced Chi-Sqr	99.11779		
Adj. R-Square	0.97671		
		Value	Standard Error
	y0	3.00133	0.72967
	xc	875.11741	0.14239
	w	22.08562	0.29893
	A	6943.77945	88.59232
	sigma	11.04281	0.14946
	FWHM	26.00383	0.35196
	Height	250.85711	2.84848

Fig. S4 E(LO) peak of sample 1 in Raman spectra. Red line is fitted curve. Right table lists our fitted data.

References

1. M. D. Fontana, P. Bourson, Microstructure and defects probed by Raman spectroscopy in lithium niobite crystals and devices. Appl. Phys. Rev., 2015, 2, 040602.

2. V. Caciuc, A. V. Postnikov, G. Borstel, Ab initio structure and zone-center phonons in $LiNbO_3$. Phys. Rev. B 2000, 61, 8806.