Supplementary Materials for

Improved performance of Li-rich cathode materials by relaxing internal stress and promoting grain growth

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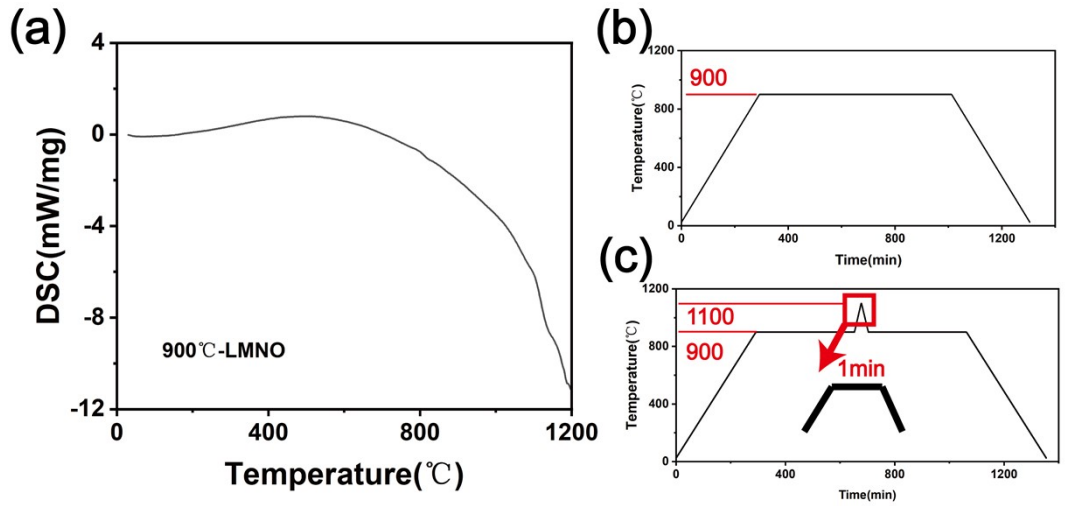


Figure S1 (a) The DSC curve of LMNO; (b) The schematic diagram of the heat treatment process for 900℃-LMNO and 900℃-Zr0.75%; (c) The schematic diagram of the heat treatment process for 1100℃-Zr0.75%.

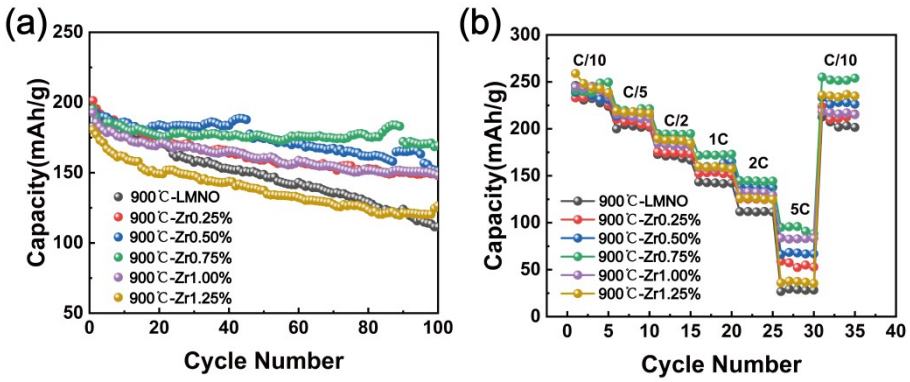


Figure S2 (a) The cyclic performance and (b) rate capability of Zr doping with different concentrations

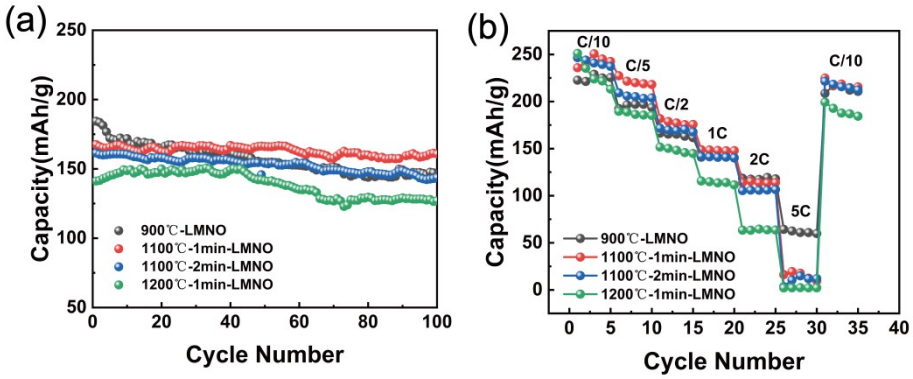


Figure S3 (a) The cyclic performance and (b) rate capability of LMNO under different thermal shock processes

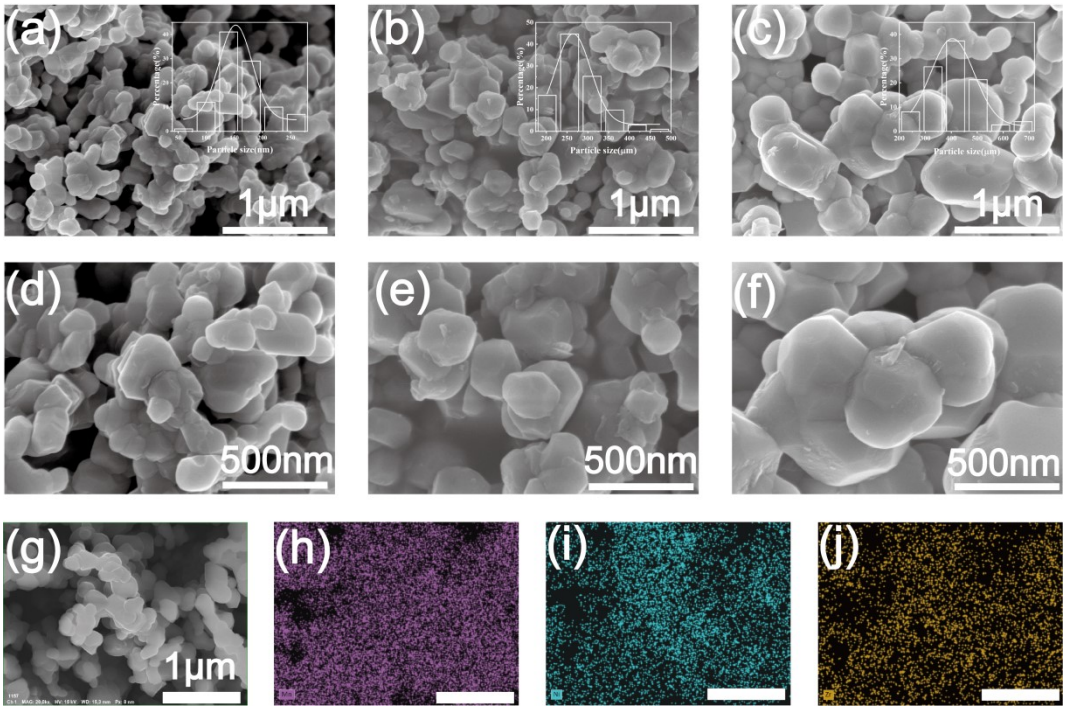


Figure S4 The SEM image of (a, d) 900℃-LMNO, (b, e) 900℃-Zr0.75% and (c, f) 1100℃-Zr0.75%；(g~j) The EDS image of 1100℃-Zr0.75%.

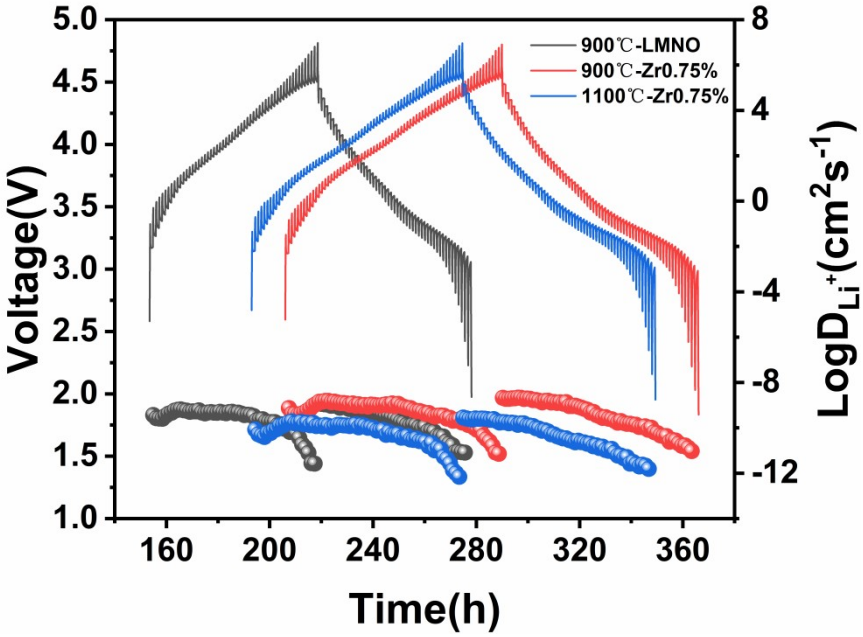


Figure S5 The gitt results of 900℃-LMNO, 900℃-Zr0.75% and 1100℃-Zr0.75%

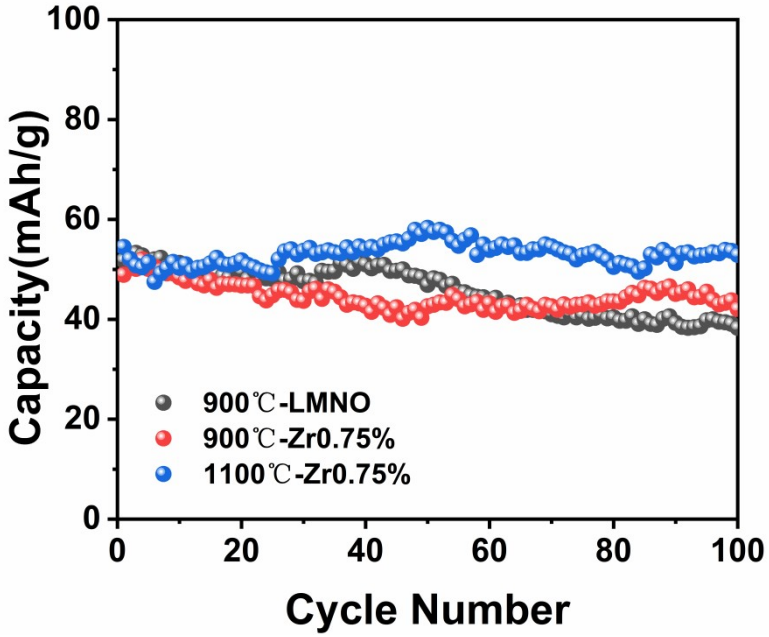


Figure S6 Full-cell testing results of 900℃-LMNO, 900℃-Zr0.75% and 1100℃-Zr0.75%

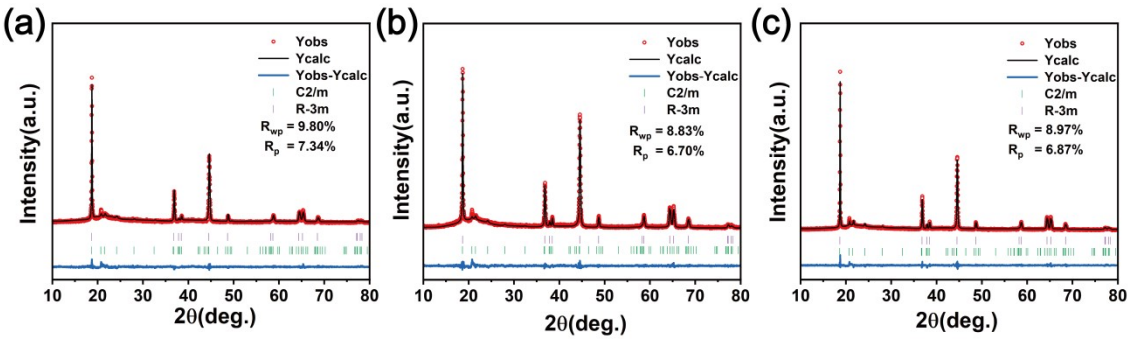


Figure S7 (a~c) The XRD Rietveld refinement results of 900℃-LMNO,900℃-Zr0.75% and 1100℃-Zr0.75%.

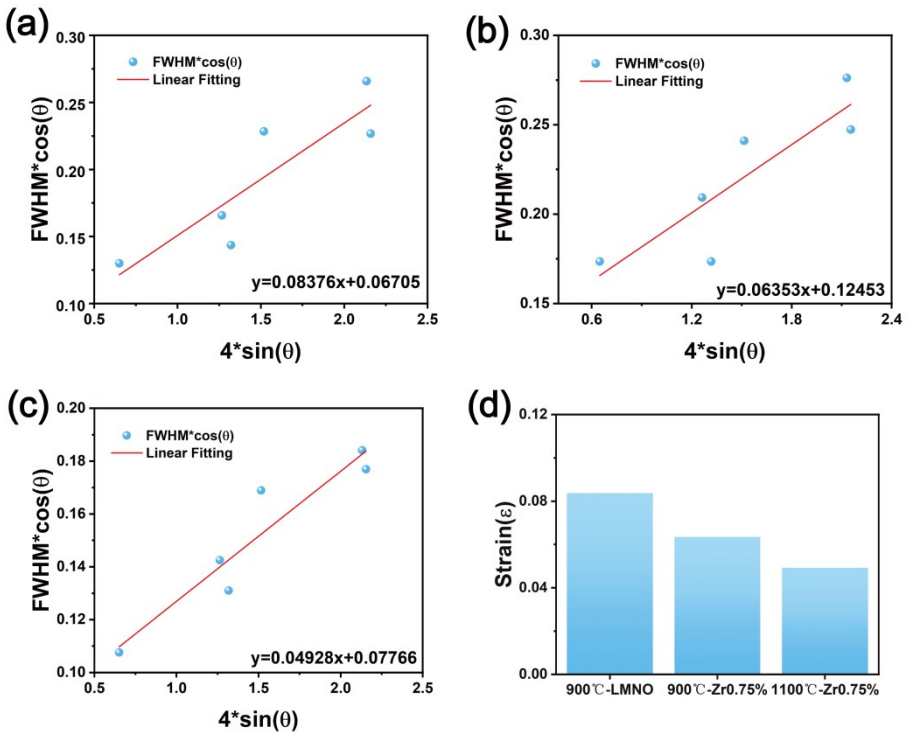


Figure S8 (a~c) The W-H method fitting results of XRD pattern for 900℃-LMNO,900℃-Zr0.75%, 1100℃-Zr0.75%; (d) The microscopic strain bar charts of three samples.

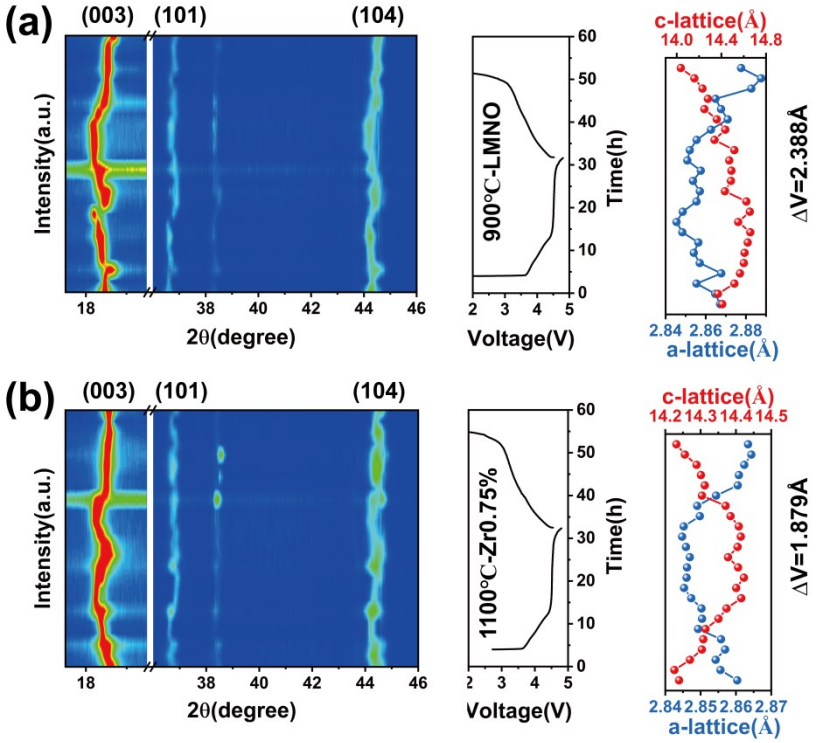


Figure S9 The ex situ XRD results of (a) 900℃-LMNO and (b) 1100℃-Zr0.75%

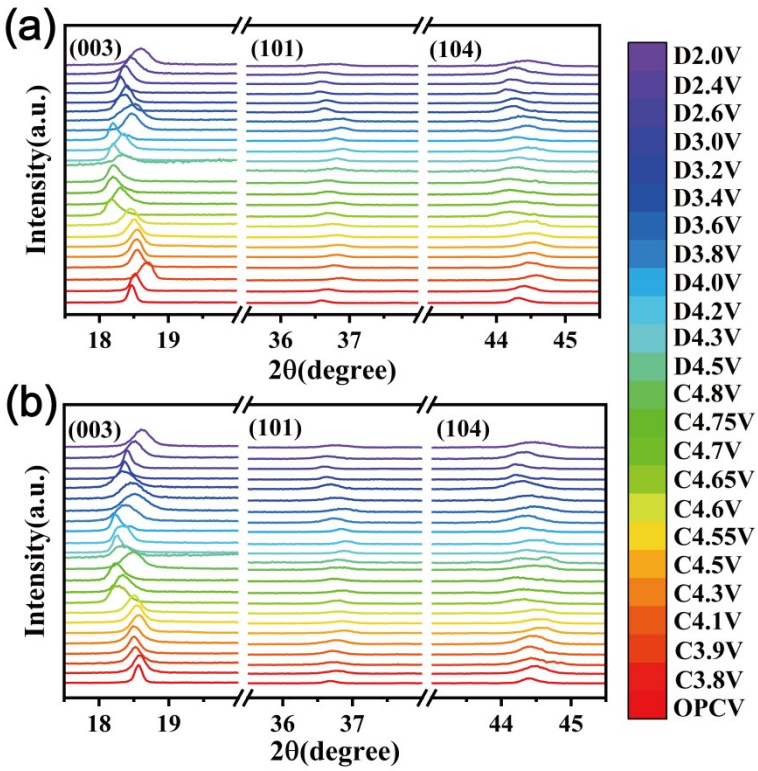
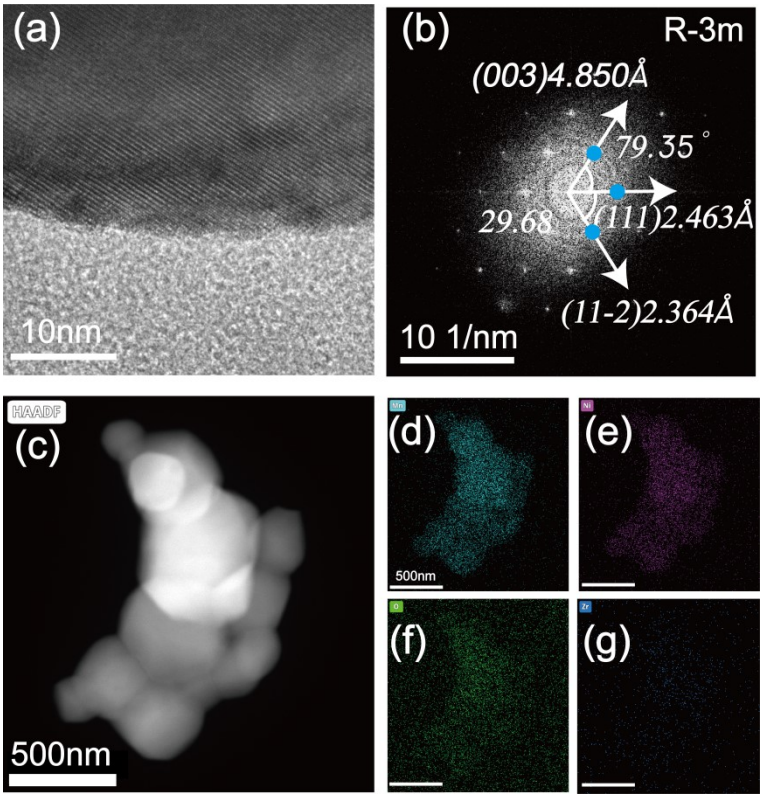
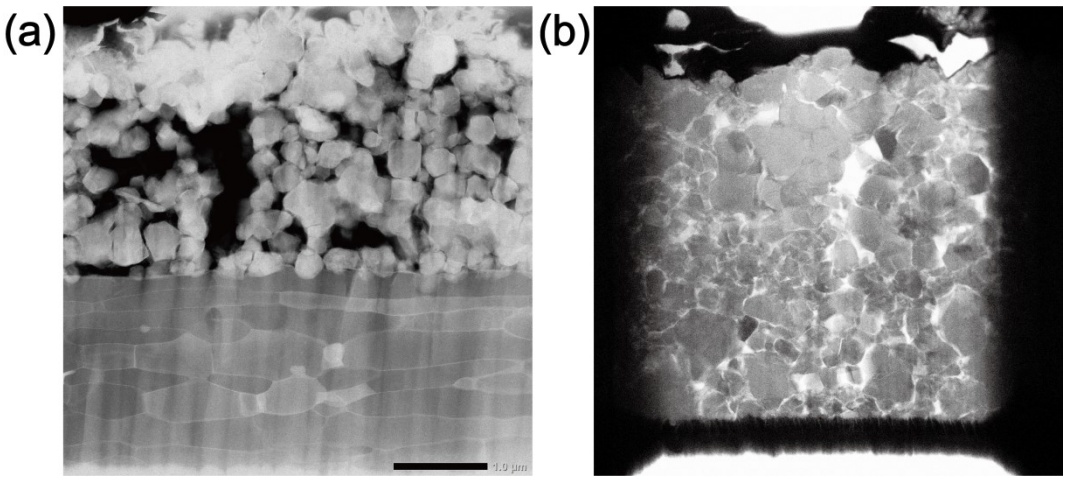


Figure S10 The XRD results of (a) 900℃-LMNO and (b) 1100℃-Zr0.75% at different voltages



FigureS11 The HRTEM image and mapping result of 1100℃-Zr0.75%.



FigureS12 The FIB results of samples

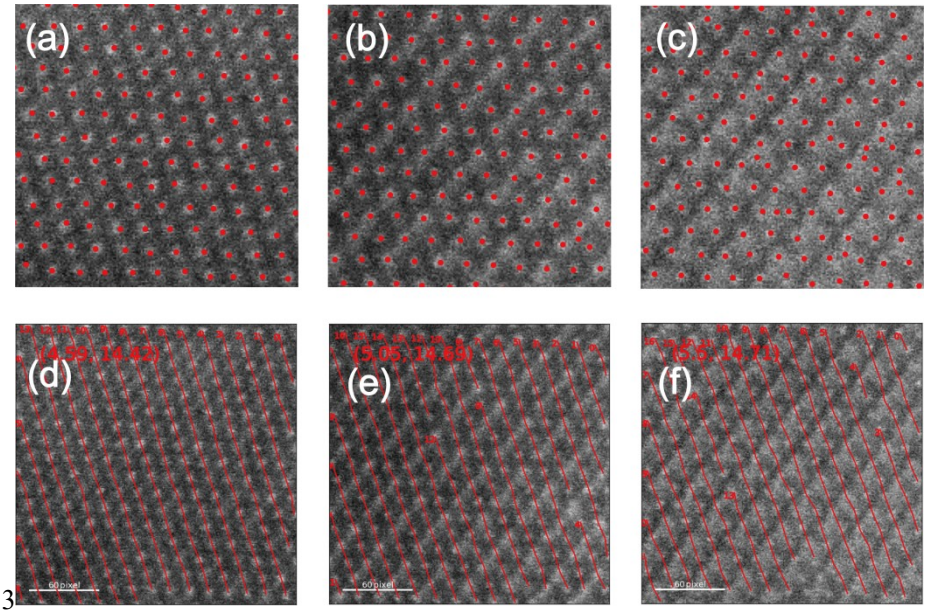


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Figure S13 The calibration of atomic columns in different regions

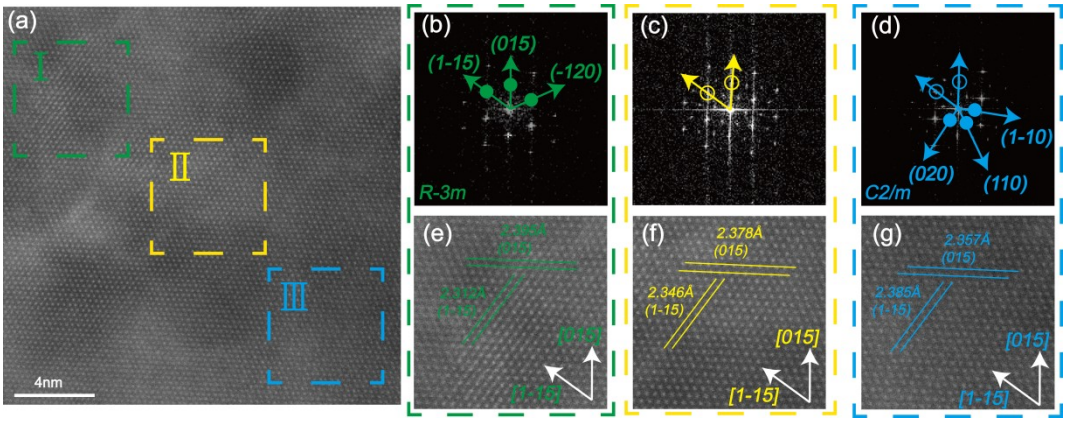

Figure S14 The AC-TEM image of 1100℃-Zr0.75%

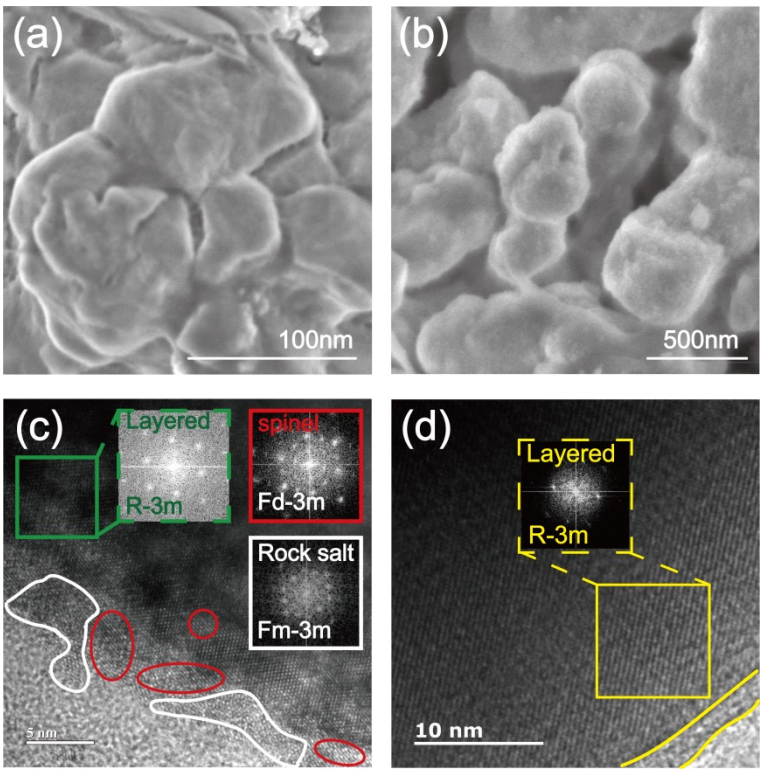

Figure S15 The SEM and TEM of (a, c) 900℃-LMNO and (b, d) 1100℃-Zr0.75% after cycling

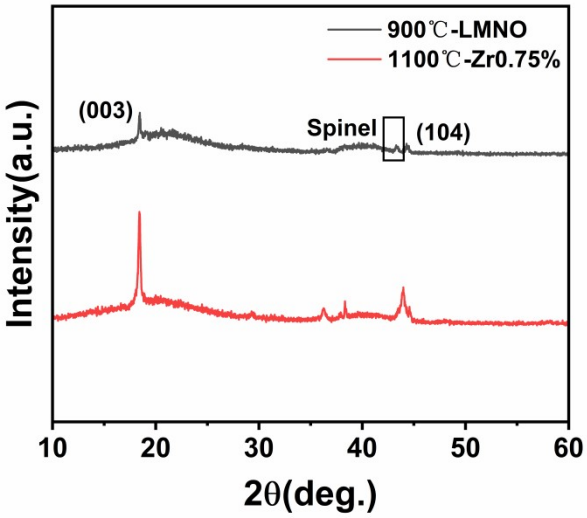

Figure S16 The XRD of 900℃-LMNO and 1100℃-Zr0.75% after cycling

Table S1 The electrochemical performance of LMNO with thermal shock

	Inital capacity(mAh/g)	Capacity after cycling(mAh/g)	Capacity retention(%)	5 C capacity(mAh/g)
900℃-LMNO	184.4	144.3	78.3	64.2
1100℃-1min-LMNO	167.5	160.8	96.0	19.4
1100℃-2min-LMNO	161.4	143.7	89.1	14.9
1200℃-1min-LMNO	141.2	127.0	89.9	2.3

Table S2 The electrochemical performance of LMNO with Zr^{4+} doping

	Inital capacity(mAh/g)	Capacity after cycling(mAh/g)	Capacity retention(%)	5 C capacity(mAh/g)
900℃-Zr0.00%	183.0	111.5	60.9	63.7
900℃-Zr0.25%	201.3	147.9	73.5	67.9
900℃-Zr0.50%	195.4	151.2	77.4	67.8
900℃-Zr0.75%	195.6	169.3	86.6	95.9
900℃-Zr1.00%	192.6	148.3	76.9	82.8
900℃-Zr1.25%	180.5	126.4	70.0	37.4

Table S3 The ICP result of 900℃-LMNO,900℃-Zr0.75% and 1100℃-Zr0.75%.

Sample	The actual molar ratio			
	Li	Mn	Ni	Zr
900℃-LMNO	1.204572199	0.59575914	0.199668661	/
900℃-Zr0.75%	1.221491846	0.578664678	0.192407529	0.007435947
1100℃-Zr0.75%	1.216175614	0.585172272	0.191314981	0.007337133

Table S4 The XRD Rietveld refinement results of 900℃-LMNO,900℃-Zr0.75% and 1100℃-Zr0.75%.

		900℃-LMNO	900℃-Zr0.75%	1100℃-Zr0.75%
Rietveld factor	R_{wp}	9.80%	8.83%	8.97%
	R_p	7.34%	6.70%	6.87%
Wt%	R-3m	56.88	54.782	65.985
	C2/m	43.12	45.218	34.015
R-3m	a	2.85473	2.85966	2.863394
	b	2.85473	2.85966	2.863394
	c	14.23096	14.252257	14.266562
	c/a	4.985045871	4.983899135	4.982395716
	V	100.437	100.935	101.301
C2/m	a	4.95542	4.994078	4.965401
	b	8.55056	8.543277	8.57469
	c	5.02225	5.038775	5.049073
	V	200.96	203.111	202.959

Table S5 The W-H method fitting results of 900℃-LMNO.

No.	2θ	FWHM	4sinθ	FWHM*cosθ
1	18.71981	0.13173	0.650542117	0.129976175
2	36.89916	0.17471	1.265880054	0.165730345
3	38.54171	0.15212	1.320137044	0.143596557
4	44.61947	0.24686	1.518453418	0.228381352
5	64.49909	0.31431	2.134431199	0.265822044
6	65.34187	0.26929	2.159253478	0.226684209

Table S6 The W-H method fitting results of 900℃-Zr0.75%.

No.	2degree	FWHM	4sin	FWHM*cos
1	18.65804	0.17579	0.64841455	0.173464955
2	36.80614	0.22056	1.262799515	0.209280363
3	38.43995	0.18378	1.316783457	0.173536408
4	44.51048	0.26042	1.514933045	0.241020239
5	64.36485	0.32632	2.130466753	0.27618308
6	65.18599	0.29348	2.15467113	0.247262259

Table S7 The W-H method fitting results of 1100℃-Zr0.75%.

No.	2degree	FWHM	4sin	FWHM*cos
1	18.71008	0.10901	0.650206995	0.107560169
2	36.82953	0.15019	1.263574199	0.142499467
3	38.47107	0.13878	1.317809153	0.131032221
4	44.53564	0.18253	1.515745834	0.168917404
5	64.35753	0.21754	2.130250491	0.184123812
6	65.17249	0.20997	2.154274088	0.176916883