energies

MDPI

Supplementary materials

Atomic Layer Deposition of Lithium–Nickel–Silicon Oxide Cathode Material for Thin-Film Lithium-Ion Batteries

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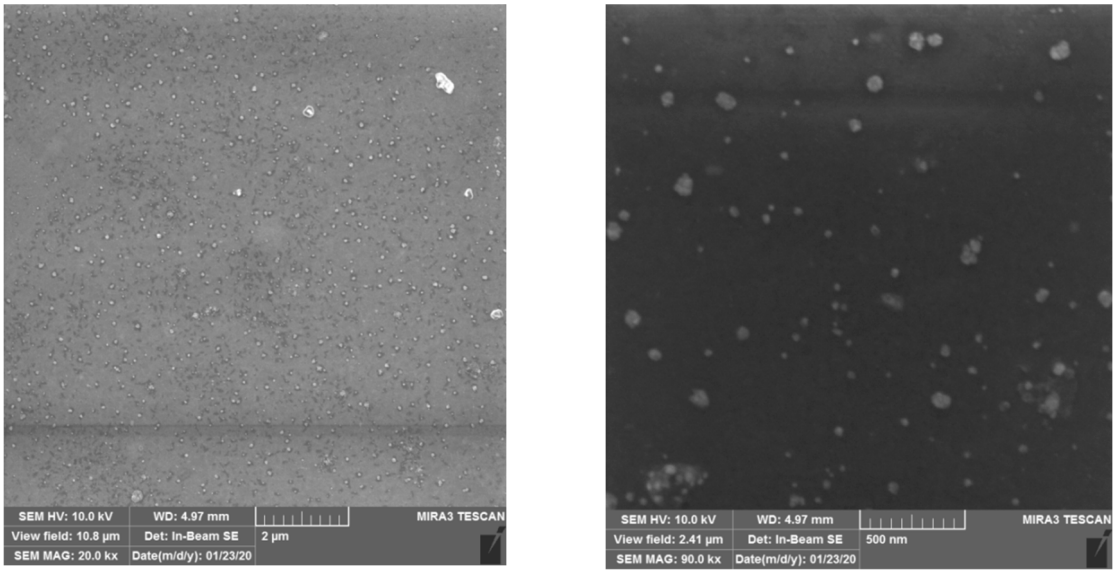
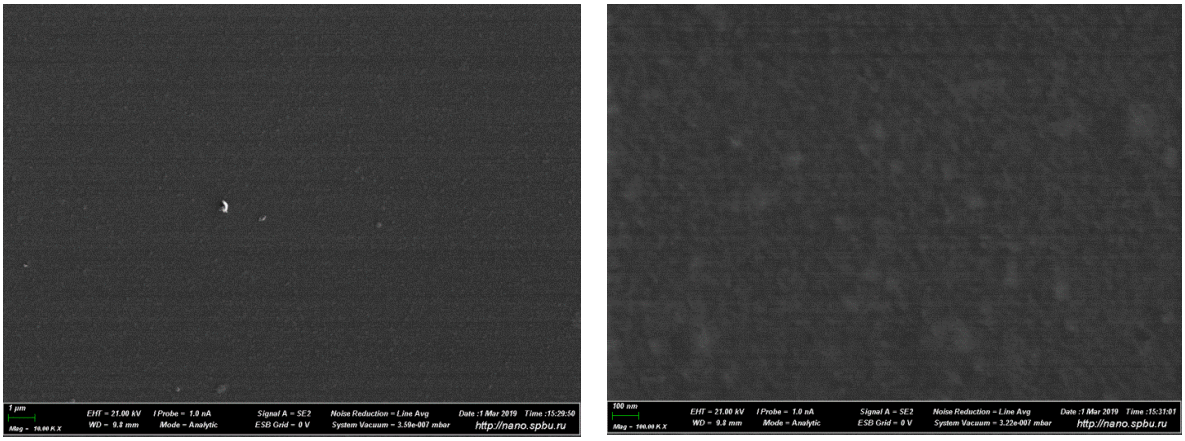
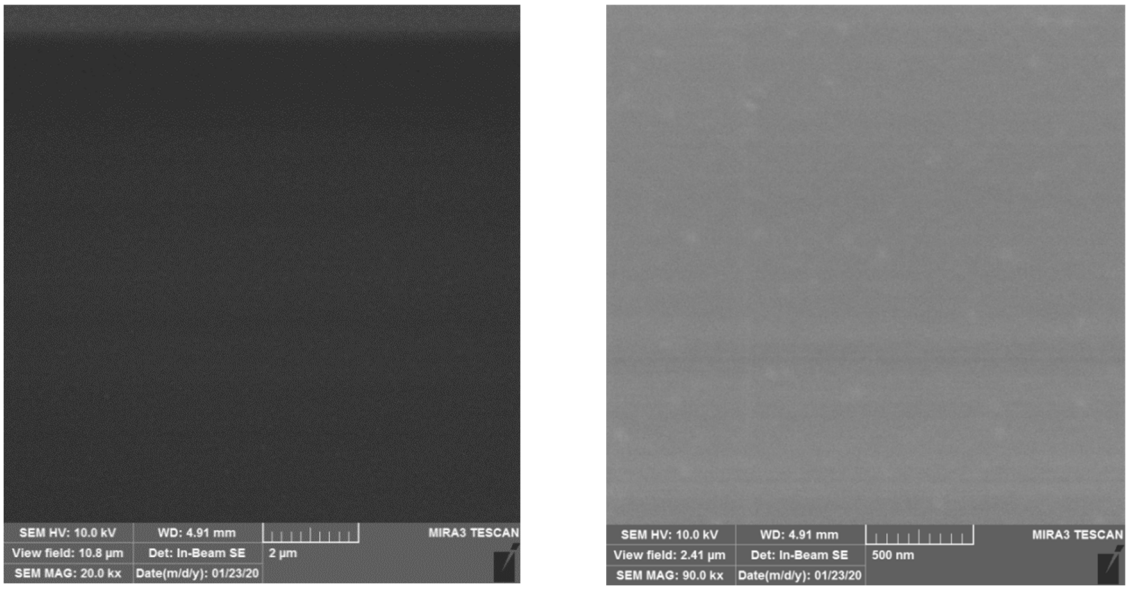


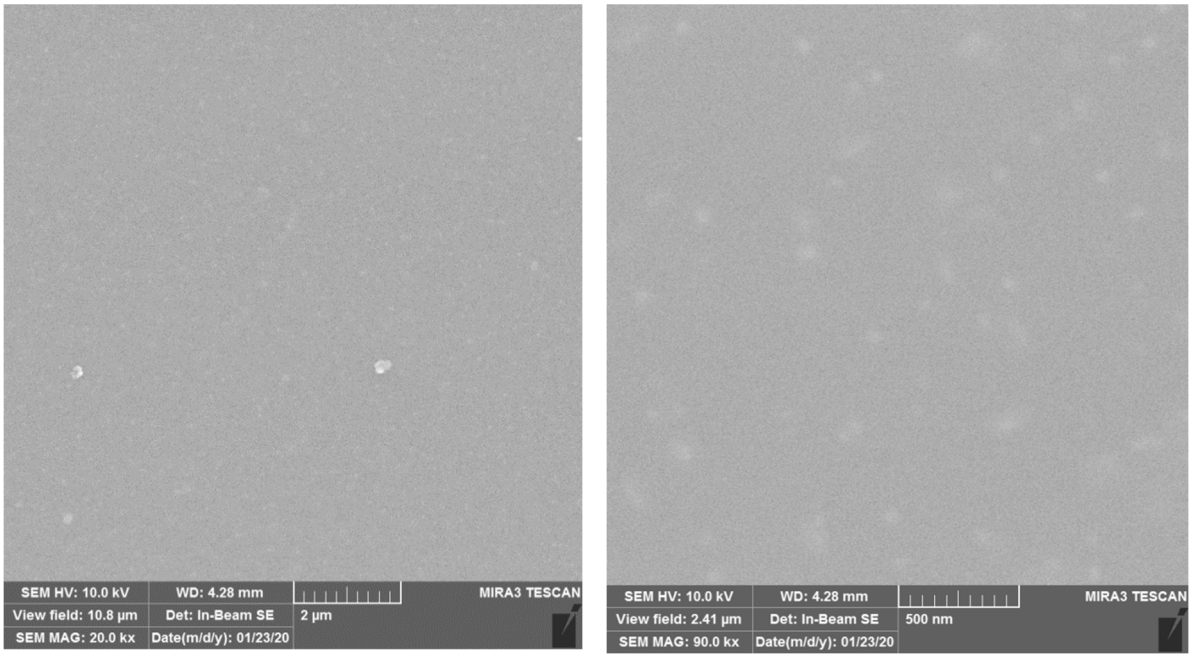
LNO-1/10



LNO-1/3



LNO-1/2



LNO-1/1

Figure S1. Plan-view SEM images of the surface of the samples LNO-1/10, LNO-1/3, LNO-1/2, LNO-1/1.

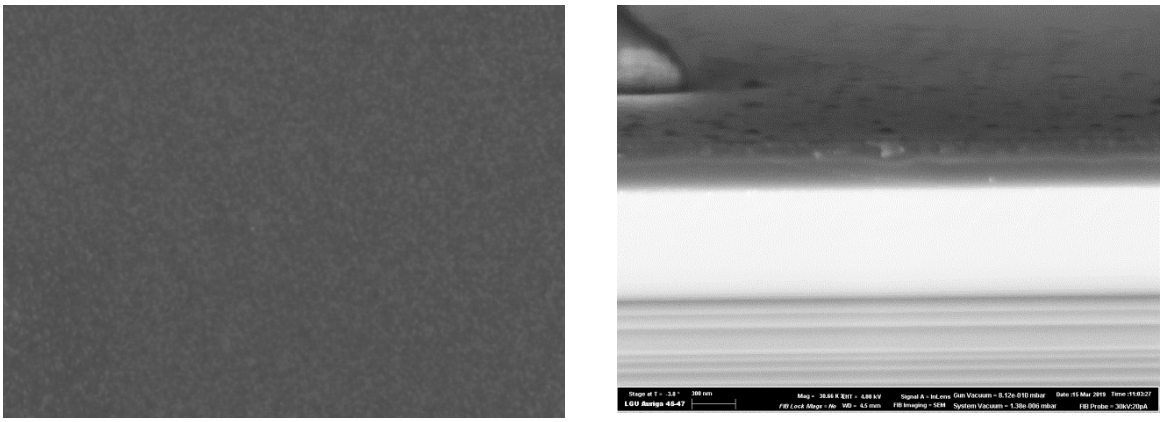


Figure S2. Plan-view (**a**) and cross-sectional (**b**) SEM images of sample LNO-1/3.

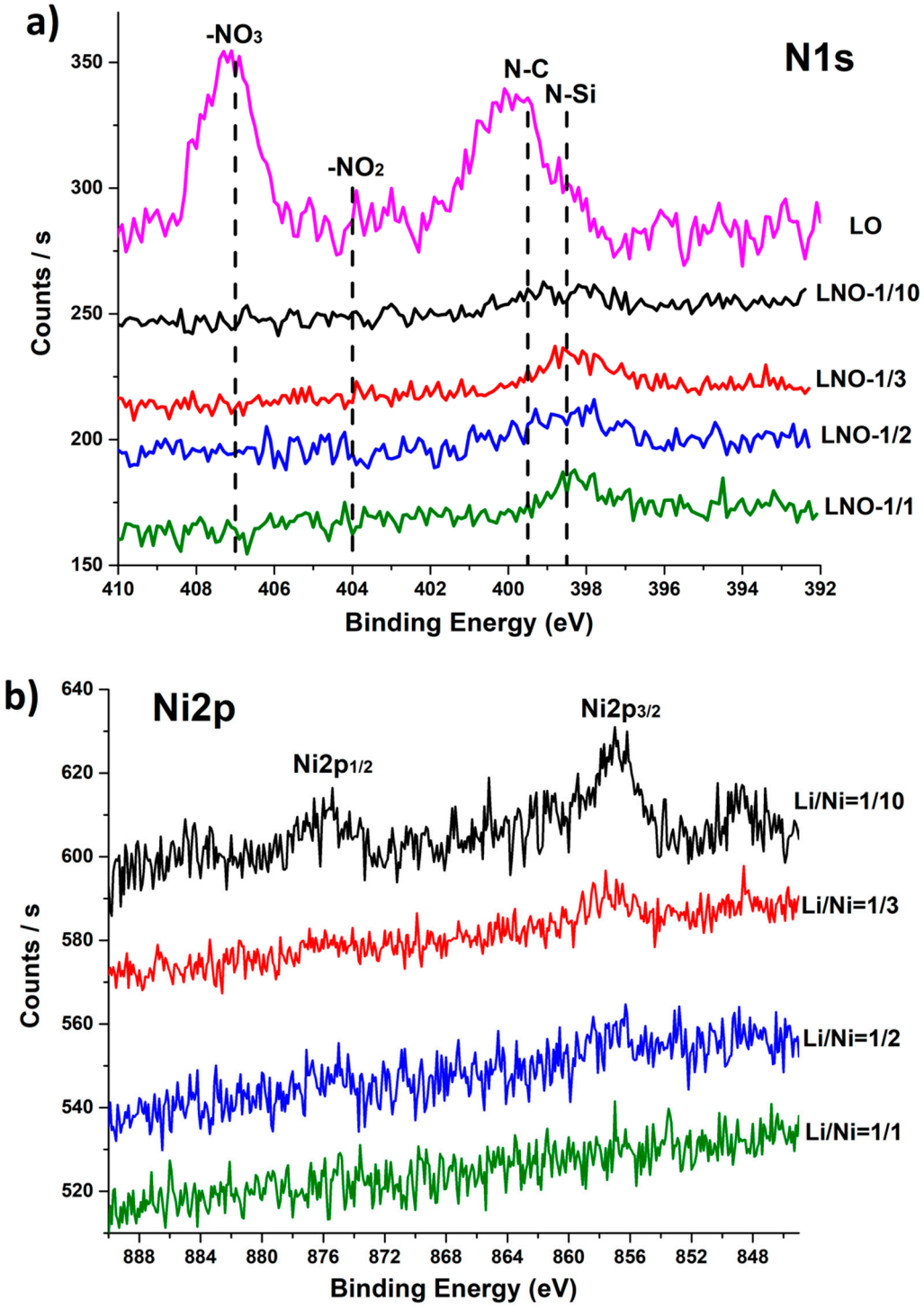


Figure S3. X-ray photoelectron (XPS) N1s (**a**) and Ni2p (**b**) spectra of LNO samples.

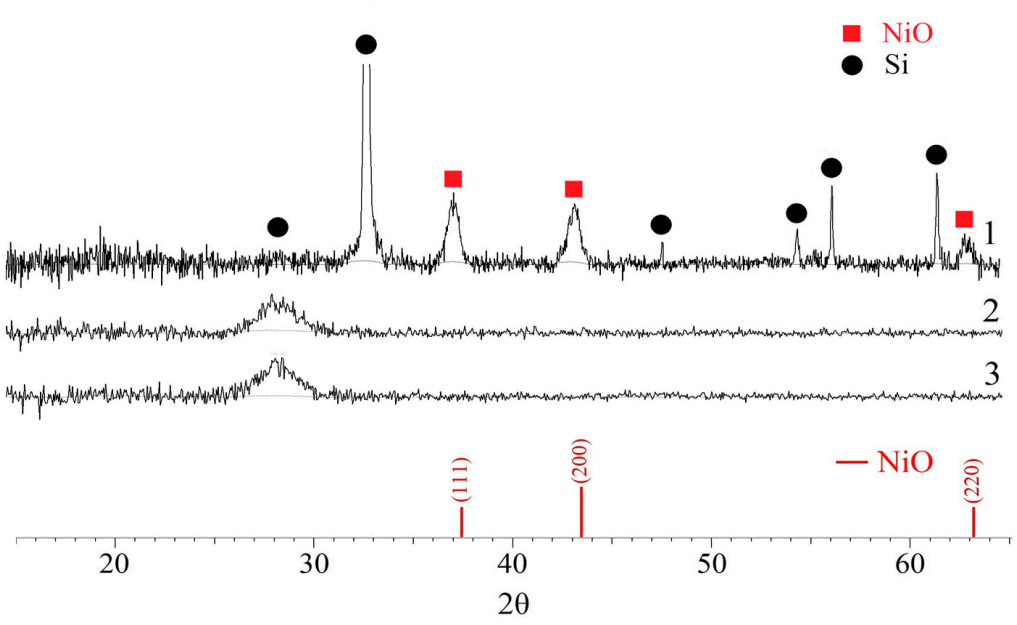


Figure S4. Grazing incidence XRD of as-deposited NO –(1), LNO-1/10 – (2), and LNO-1/3 – (3). The NiO cell parameter (a) calculated by the Rietveld method was 0.4168 nm, which is close to the value of bulk NiO: 0.418 nm (ICSD file no. 61324 (2006)).

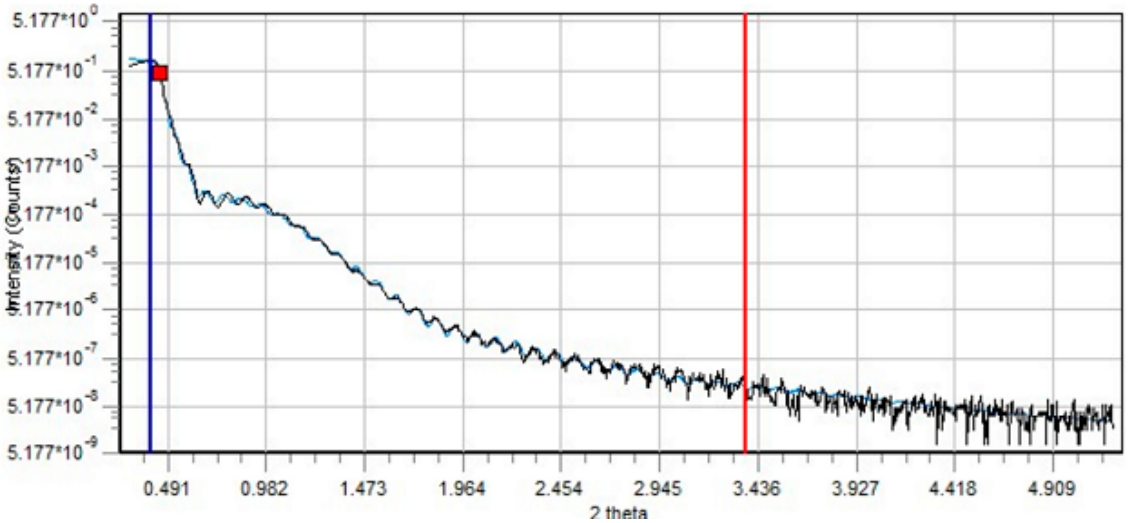


Figure S5. X-ray reflectometry (XRR) curve of LNO-1/3.

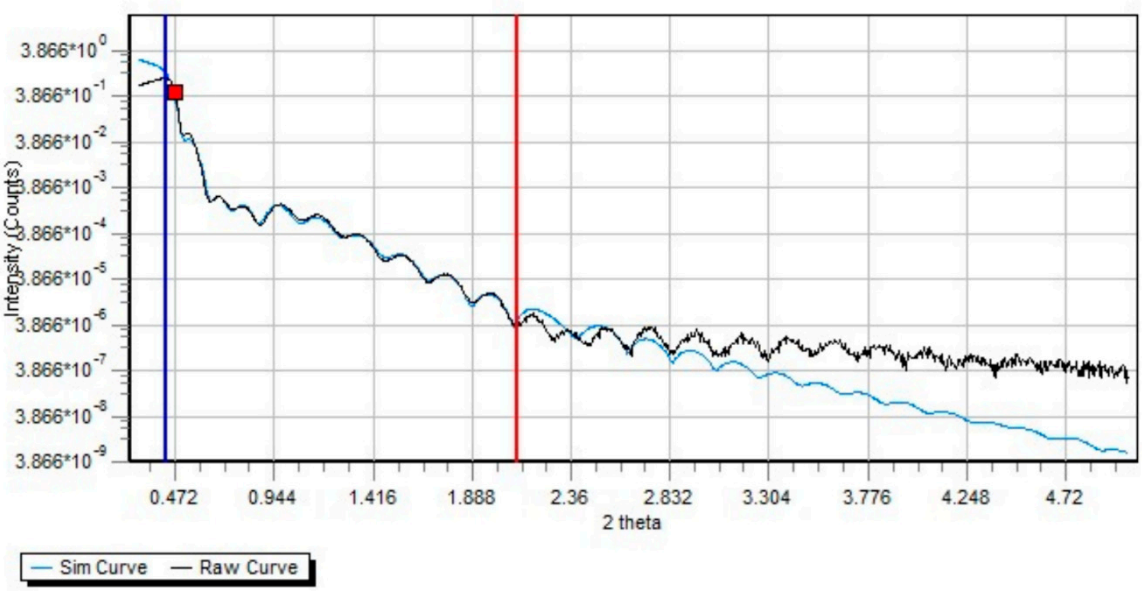


Figure S6. X-ray reflectometry (XRR) curve of LNO-1/10.

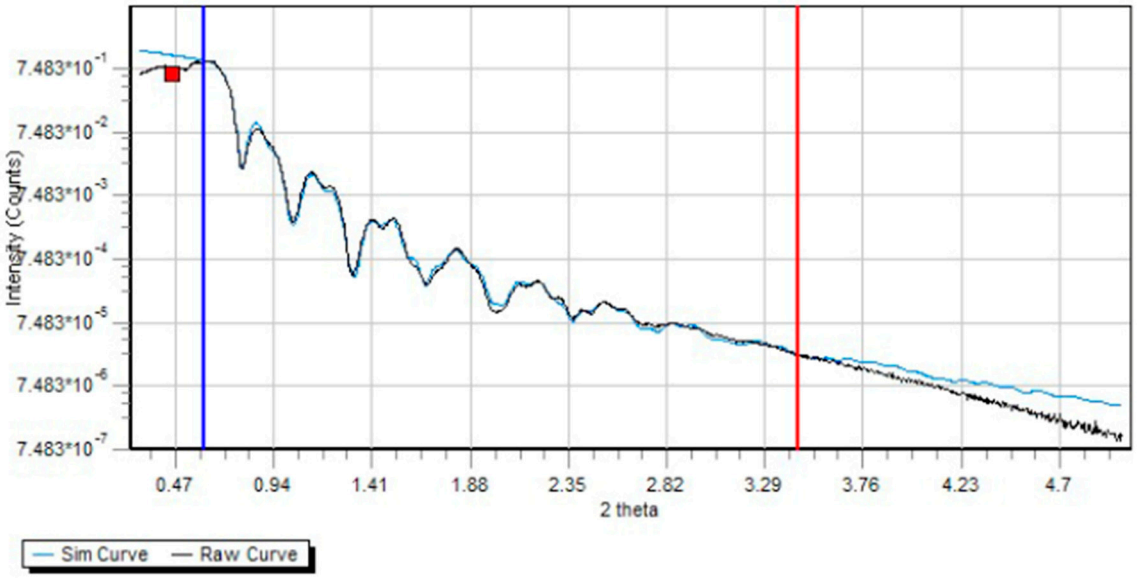


Figure S7. X-ray reflectometry (XRR) curve of LNO-M.

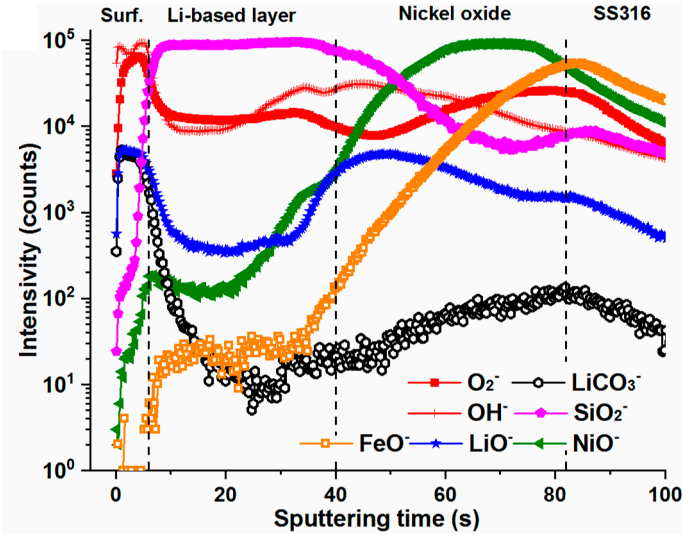


Figure S8. Time-of-flight secondary-ion-mass spectroscopy (TOF-SIMS) depth profiles of the negative ions of LNO-M.

Table S1. Results of X-ray photoelectron (XPS) depth profiling of LNO-M.

Sputtering time, s	C, %	O, %	Li, %	Si, %	Ni, %
0	39.91	31.45	28.64	-	-
15	21.15	42.30	33.44	3.11	-
45	1.76	52.65	27.45	18.14	-
110	-	57.46	17.89	24.51	0.13
155	-	56.36	19.31	24.22	0.11
210	-	56.73	20.02	23.14	0.11
255	-	55.15	22.64	22.09	0.12
315	-	53.95	24.95	21.01	0.09
675	-	45.74	40.50	12.35	1.41
1035	-	52.05	-	1.63	46.32

Table S2. Results of X-ray photoelectron spectroscopy (XPS) depth profiling of LNO-M-800.

Sputtering Time, s	C, %	O, %	Li, %	Si, %	Ni, %	F, %	Cr, %	Fe, %
Air, 0	40.57	12.88	35.20	1.67	1.20	6.85	0.56	1.06
30	3.57	11.73	68.84	0.55	3.67	3.50	0.92	7.22
150	1.94	11.66	72.62	0.26	3.88	0.63	1.35	7.67
300	1.20	12.22	72.95	0.38	3.38	0.21	1.83	7.84
450	1.15	12.33	73.38	0.41	2.80	0.16	2.32	7.46
600	1.11	12.99	72.76	0.75	2.37	0.12	2.81	7.09

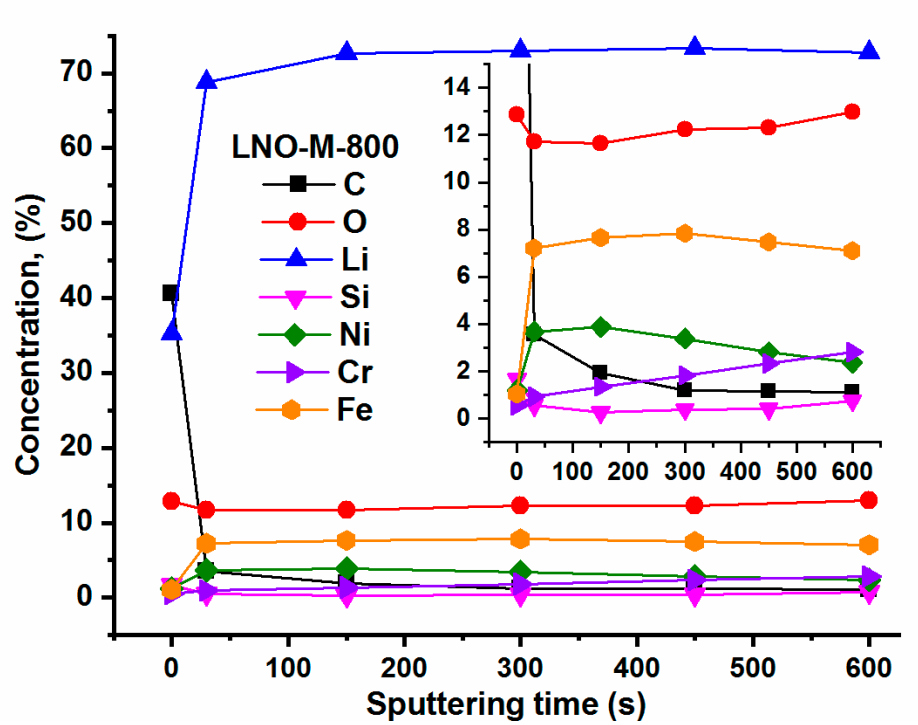


Figure S9. X-ray photoelectron spectroscopy depth profiles of the LNO-M-800.

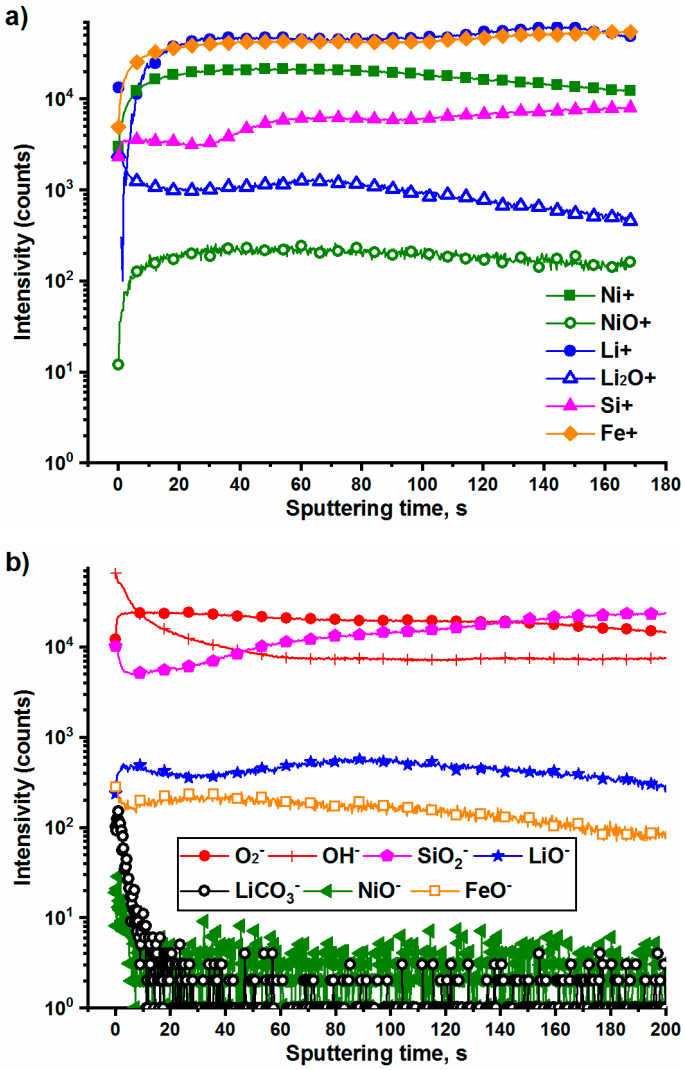


Figure 10. Time-of-flight secondary-ion-mass spectroscopy (TOF-SIMS) depth profiles of the LNO-M-800 (**a**) positive ions, (**b**) negative ions.

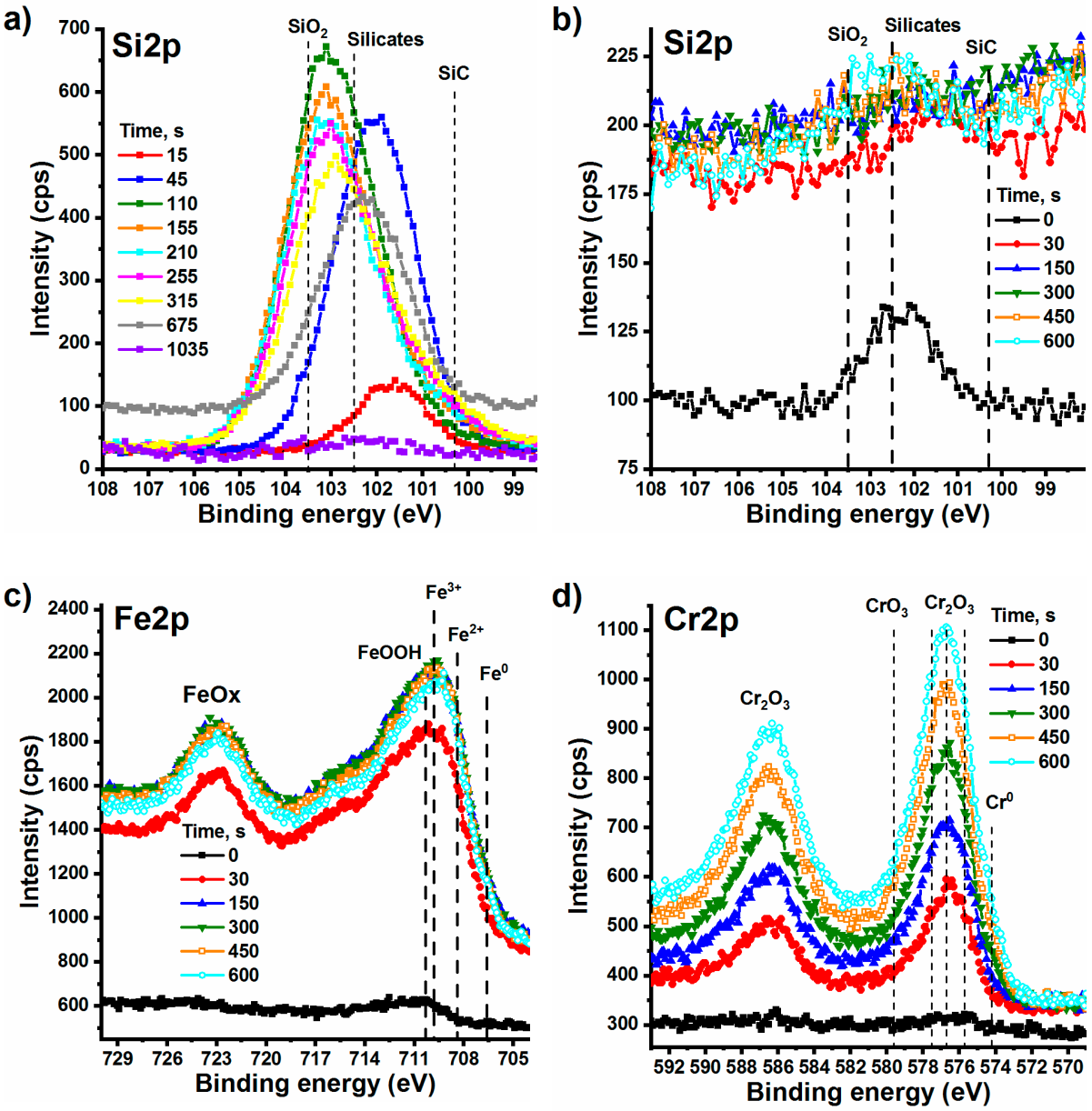
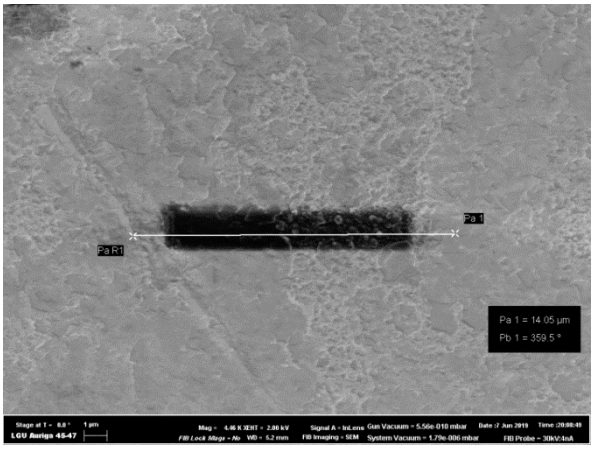
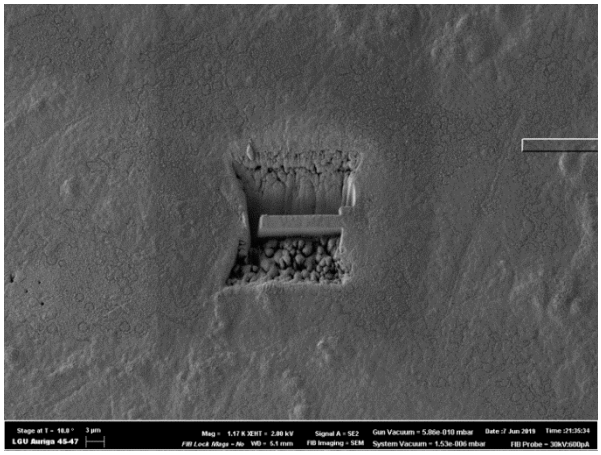


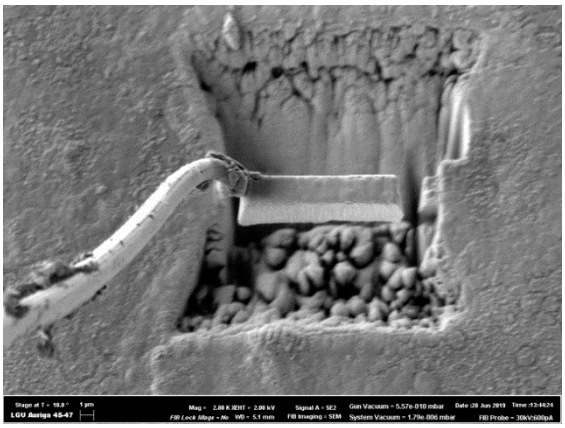
Figure S11. X-ray photoelectron (XPS) Si2p spectra of LNO-M – (**a**), Si2p spectra of LNO-M-800 – (**b**), Fe2p spectra of LNO-M-800 – (**c**), Cr2p spectra of LNO-M-800 – (**d**).



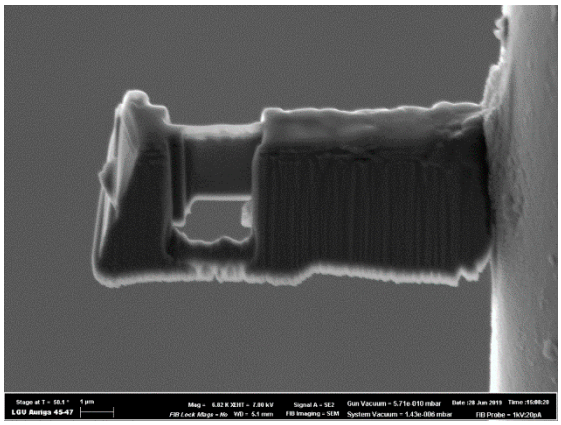
SEM image of area selected for lamella preparation and platinum deposition to prevent the structural damage in subsurface layer



SEM image of bulk-out process and perimeter cutting of lamella



SEM image of the micromanipulator which is brought to the lamella and fixed by platinum deposition. A last attaching point is cut-off and the lamella is lift-out



SEM image of the lamella fixed on TEM grid. After that a part of the lamella thinning up-to 50-100 nm. Finally, the lamella is polished at 3kV of FIB.

Figure S12. SEM images of lamella preparation.

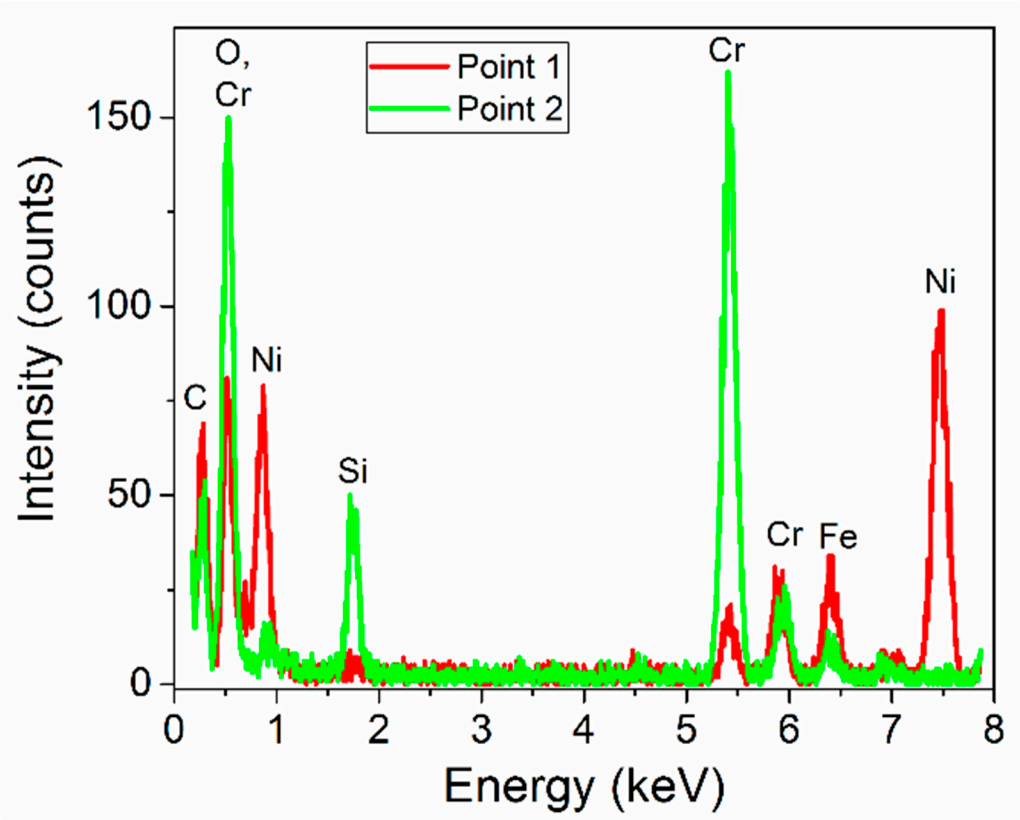


Figure S13. Energy-dispersive X-ray spectroscopy (EDX) spectra obtained in point 1 and 2 marked in Figure 10a.

Table S3. NiO and $LiNiO_2$ crystal lattice parameters.

NiO			**$LiNiO_2$**		
hkl	d, Å	Intensity, %	hkl	d, Å	Intensity, %
(111)	2.43	65	003	4.78	100
(200)	2.1	100	(101)	2.47	37
(220)	1.48	48	(104)	2.06	70
			(107)	1.59	12
			(10-8)	1.46	16
			(2-10)	1.45	16