

Supplementary Information

Role of Nanoscale-range Vanadium Treatment on LiNi_{0.8}Co_{0.15}Al_{0.05}O₂

Cathode materials for Li-ion Batteries at Elevated Temperatures

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Table S1. The comparison electrochemical performances of VNCA with other coating materials on $\text{LiNi}_{0.8}\text{Co}_{0.15}\text{Al}_{0.05}\text{O}_2$ cathodes.

Coating materials used in	Current density	Cycle performance (rate-cycle #)				Ref.
		55 °C	60 °C	-	-	
$\text{LiNi}_{0.8}\text{Co}_{0.15}\text{Al}_{0.05}\text{O}_2$		-	-	94%	1C-100	
V	1.5 mAcm⁻²					This Work
		-	-	90%	1C-200	
Mn		75%	2C-100	-	-	1
$\text{Li}_2\text{O}-2\text{B}_2\text{O}_3$		94%	1C-100	-	-	2
LiCoO_2		98%	1C-50	-	-	3
$\text{Ni}_3(\text{PO}_4)_2$		75%	1C-100	-	-	4
AlF_3		85%	1C-100	-	-	5
SiO_2	1.9 mAcm ⁻²	-	-	61%	1C-40th	6
TiO_2	1.9 mAcm ⁻²	-	-	71%	1C-40th	7

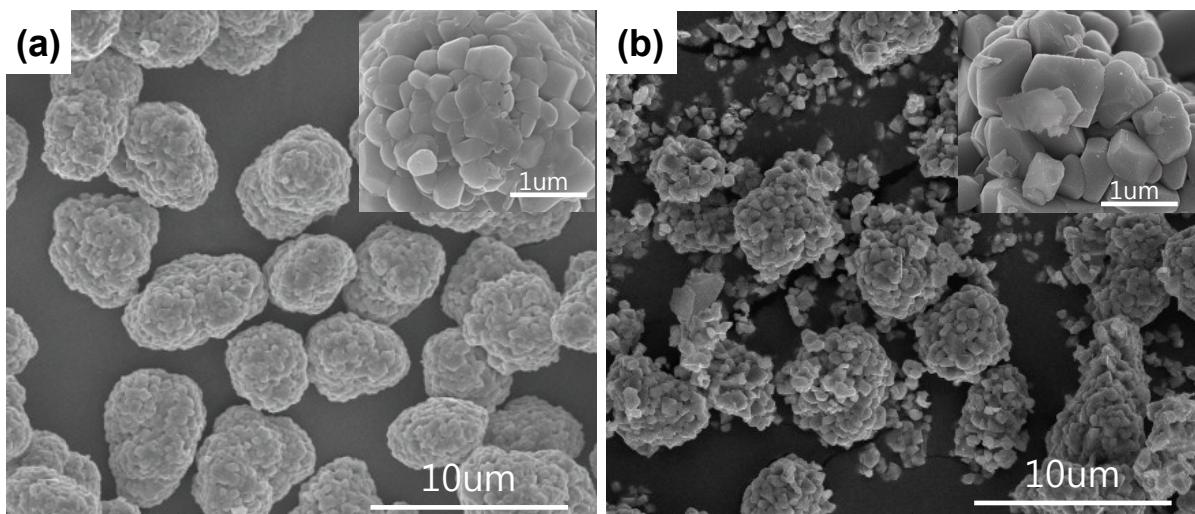


Figure S1. SEM images of (a) Pristine $\text{LiNi}_{0.8}\text{Co}_{0.15}\text{Al}_{0.05}\text{O}_2$ and (b) $\text{LiNi}_{0.8}\text{Co}_{0.15}\text{Al}_{0.05}\text{O}_2$ after annealing at $700\text{ }^\circ\text{C}$ for 5hr

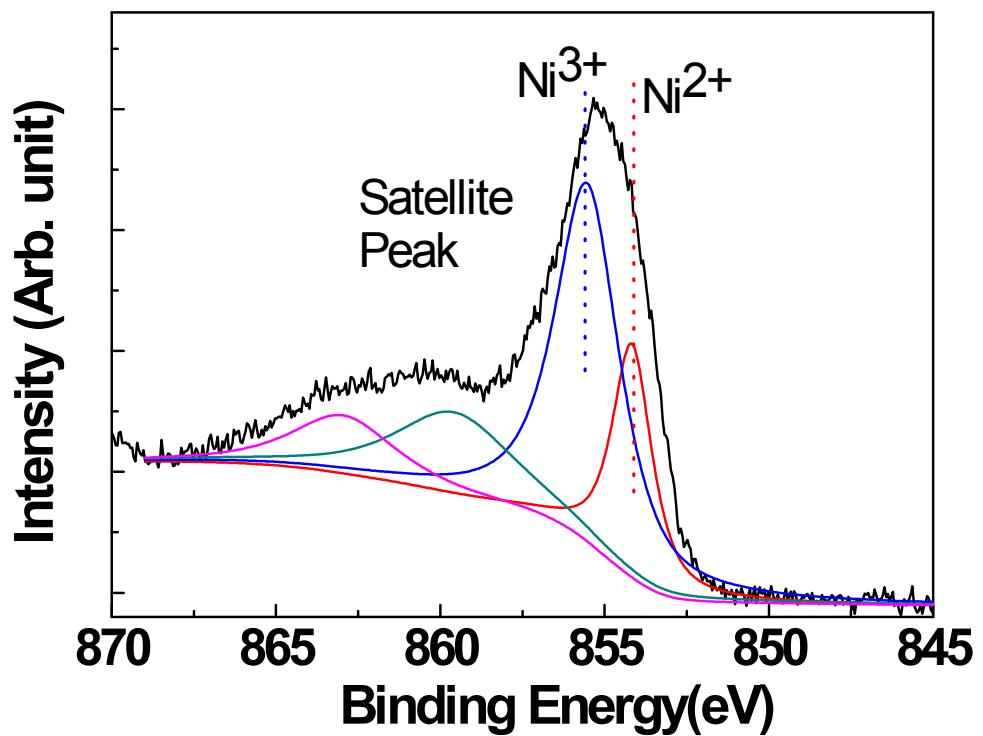


Figure S2. XPS spectrum of Ni2p_{3/2} of BNCA.

Table S2. Rietveld refinement results of BNCA and VNCA

Sample name	Lattice parameter		c/a	V [Å ³]	Ni occupancy in Li site [%]	R _{wp}	R _{exp}
	a [Å]	c [Å]					
BNCA	2.8657(1)	14.1853(2)	4.9500(1)	100.89(2)	1.20(1)	6.45	2.79
VNCA	2.8650(1)	14.1814(1)	4.9499(1)	100.81(1)	1.06(1)	4.84	2.17

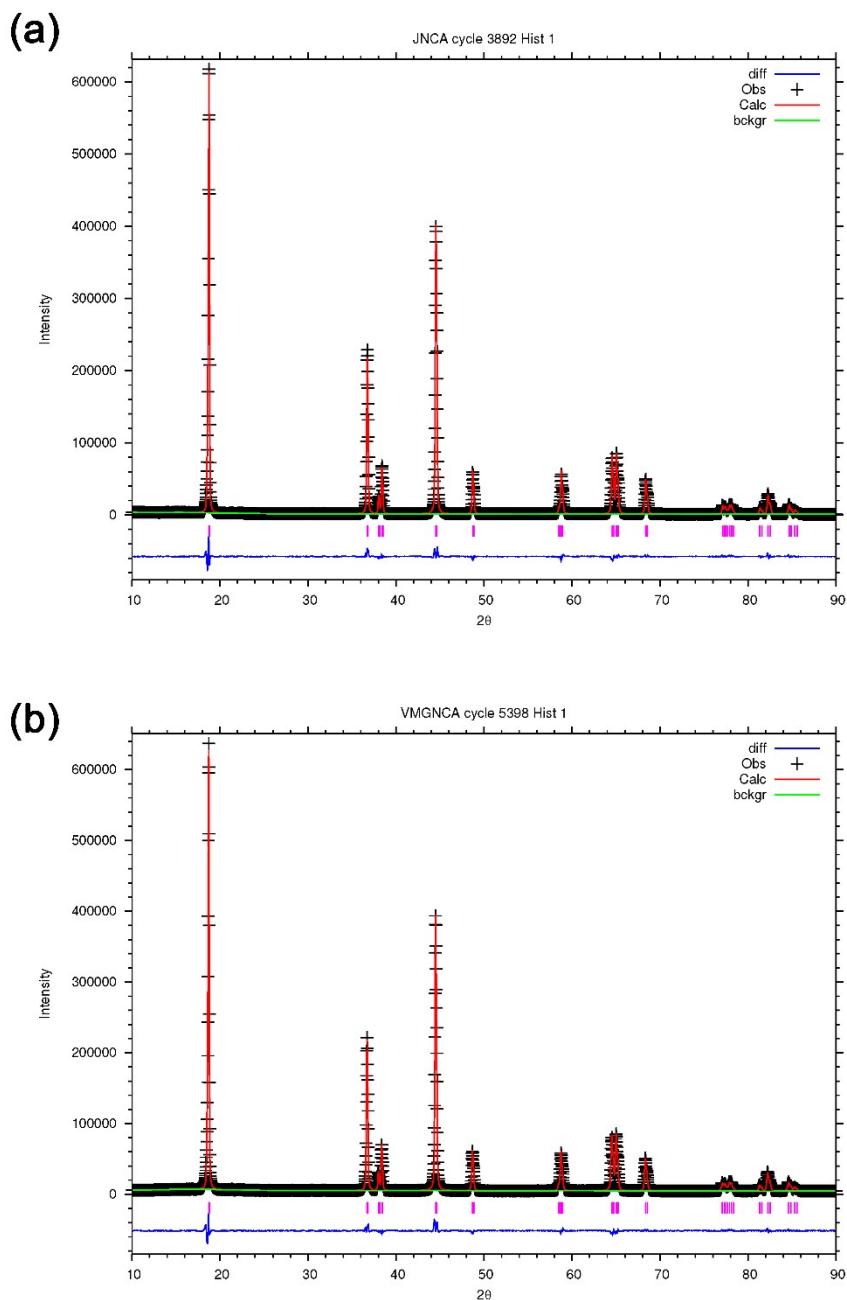


Figure S3. Rietveld Refinement of (a) BNCA and (b)VNCA.

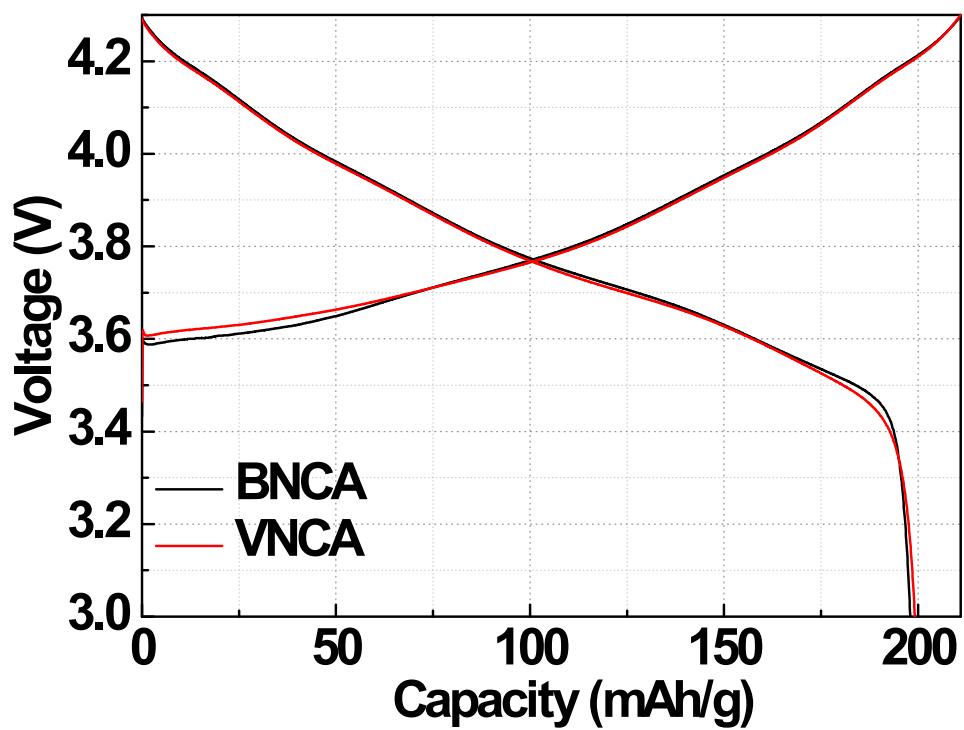


Figure S4. First charge and discharge profiles of BNCA and VNCA at 0.1C rate at 24 °C.

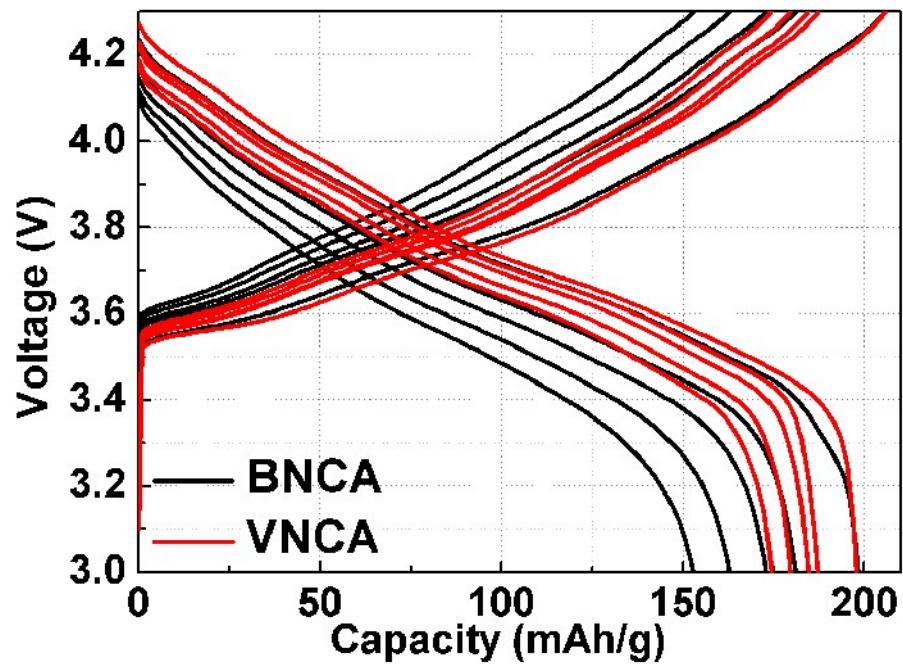


Figure S5. Voltage profiles of BNCA and VNCA at 1, 50, 100, 150, and 200 cycles.

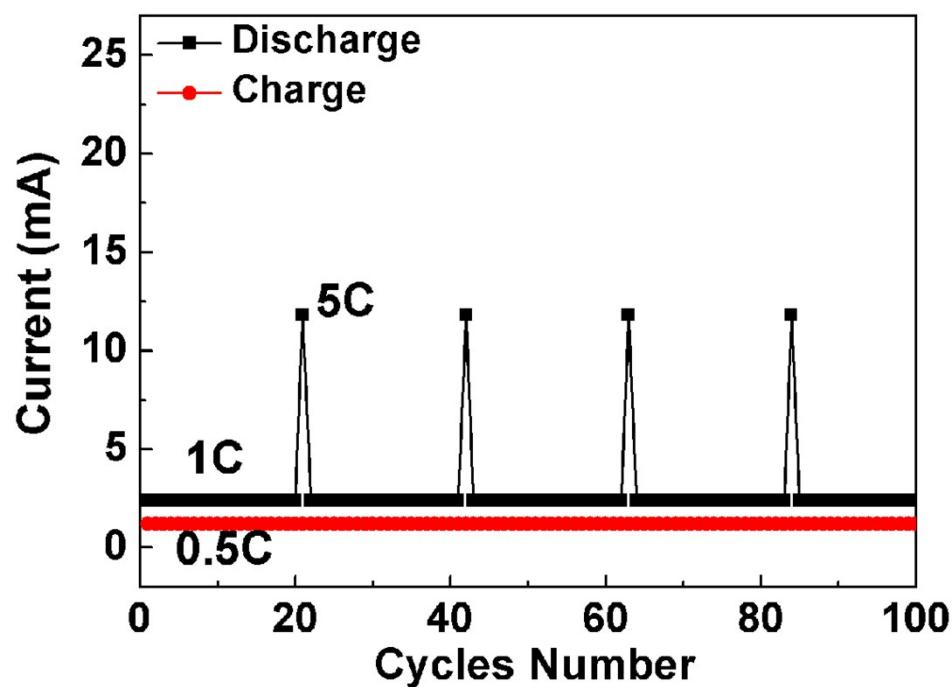
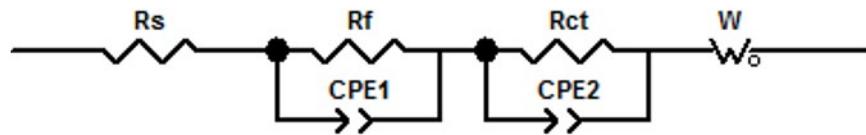


Figure S6. Current condition applied in the BNCA and VNCA cathodes in lithium half-cells (2032R). A pulse corresponding to 5 C rate was applied every 20 cycles.

(a)



(b)

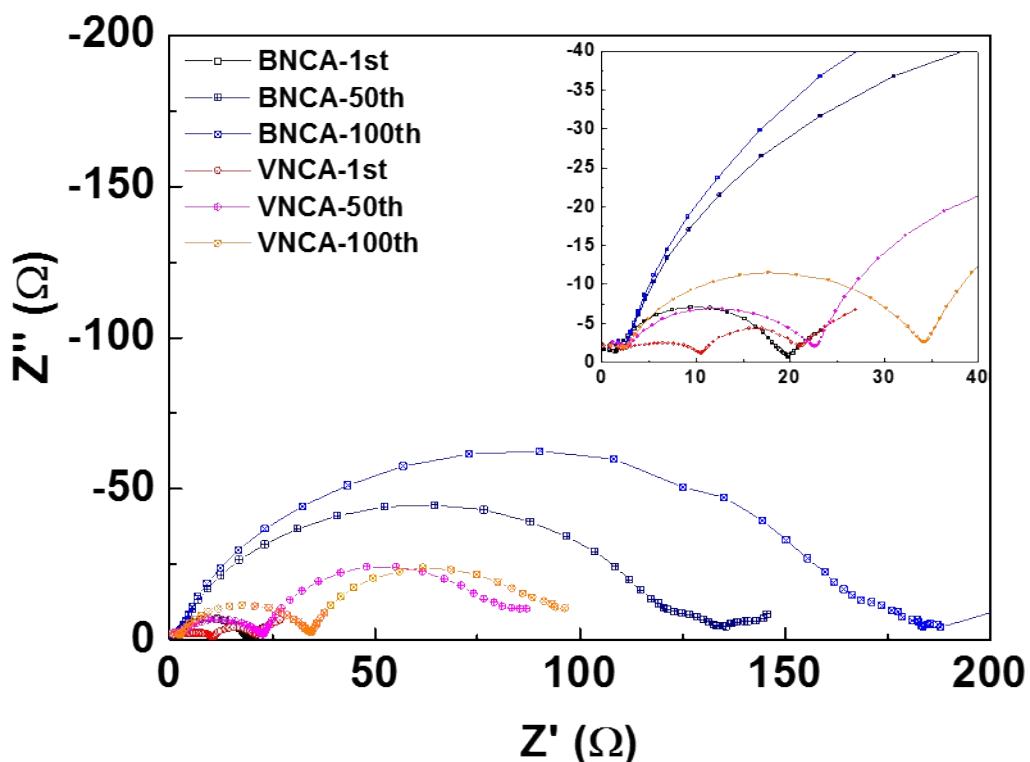


Figure S7. (a) Equivalent circuit for the electrochemical impedance of BNCA and VNCA. (b) Nyquist plots of BNCA and VNCA charged at state to 4.1 V at 60 °C with respect to cycle numbers: 1st, 50th and 100th cycle.

Table S3. Solution resistance (R_s) and sum of surface film and charge-transfer resistance (R_f+R_{ct}) of BNCA and VNCA as a function of cycle number at 60°C.

Cycle number	BNCA		VNCA	
	R_s (Ω)	R_f+R_{ct} (Ω)	R_s (Ω)	R_f+R_{ct} (Ω)
1	2	20	2	27
50	2	134	3	77
100	2	183	3	101

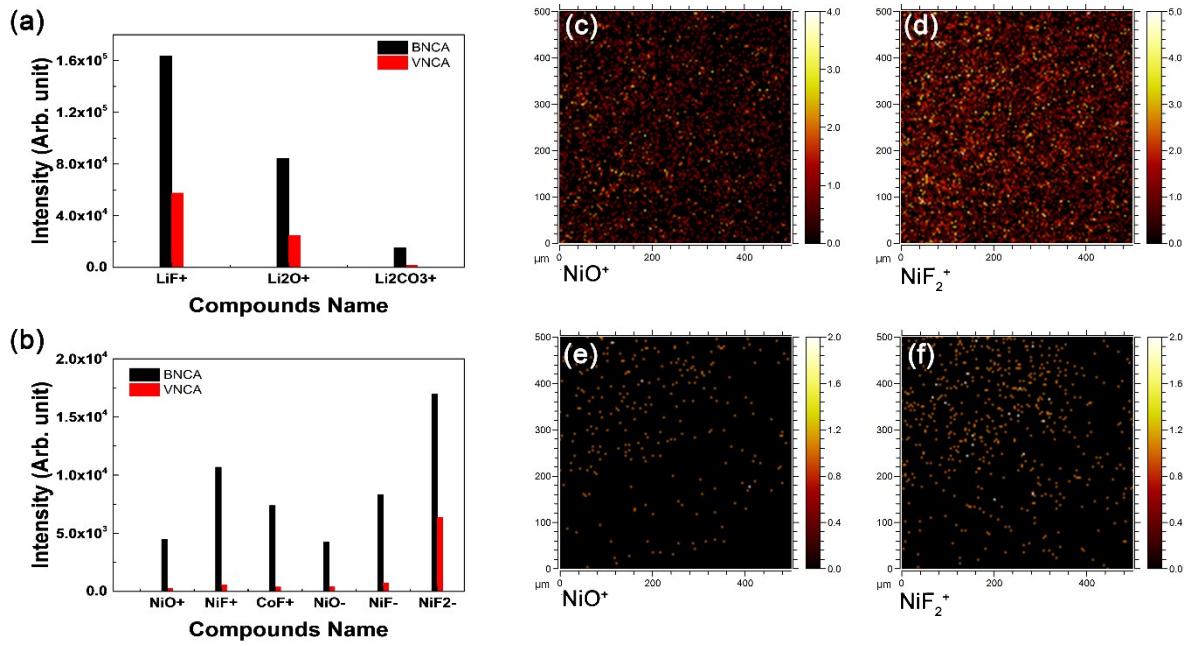


Figure S8. TOF-SIMS analysis of BNCA and VNCA electrodes after 200 cycles at 60 °C and mapping images of NiO⁺ and NiF₂⁺ in BNCA (c and d) and VNCA electrodes (e and f).

Reference

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