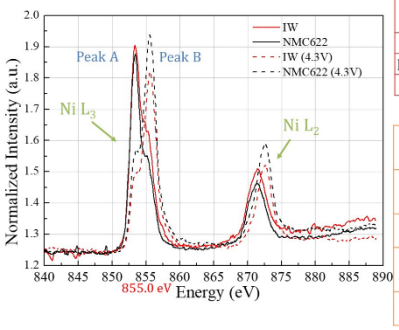
High safety self-catalyzed electrode additive for lithium-ion battery

Yung-Jen, Chang[1], Chun-Chuan Hsu[2], Nan-Hung Yeh[3], Fu-Ming Wang[3,4*]
[1] *Department of Materials Science and Engineering, National Taiwan University of Science and Technology*
[2] *Chemical Engineering, National Taiwan University of Science and Technology*
[3] *Graduate Institute of Applied Science and Technology, National Taiwan University of Science and Technology*
[4]*Sustainable Energy Center, National Taiwan University of Science and Technology*
43 Keelung Road, Section 4, Taipei 10607, Taiwan
Correspondence: mccabe@mail.ntust.edu.tw

Abstract

Rechargeable lithium-ion batteries have become the main power sources for portable electronic devices due to their high energy density and long cycle life and are actively being developed as power supplies for electric vehicles and energy storage systems. The Nickel ions plays an important role in the high energy NMC cathode system, which not only dominate the battery capacity but also influence the material thermal stability. It accelerates the battery fading and raise the risk of thermal runaway, however.

A novel oligomer electrode additive has been mixing in slurry during the electrode preparation, which can ameliorate battery performance with its special nickel trigger electrochemically atom transfer radical polymerization (e-ATRP). Several advanced in-situ and in-operando electrochemical XAS, GCMS and XRD has been introduced to observe the interaction between electrode additive and Ni-rich NMC cathode system in this work. The in-situ XAS and cycle performance of various Ni content NMC cathode material evidence that the Ni^{2+} in Ni-rich cathode material lattice will trigger the electrode additive electrochemically atom transfer radical polymerization to oxidize $Ni^{2+} \rightarrow Ni^{3+}$, and the efficacy getting significant with Ni content rising in NMC cathode materials. As the result, the additive not only help the stability of electrochemical reaction in high temperature, but also provide high coulombic efficiency.



Sample	Peak A (eV)	Peak B(eV)	A_{area}/B_{area}
NMC622 (fresh)	853.379	855.08	1.806
IW (fresh)	853.3	855.052 eV	1.28
NMC622 (4.3V)	853.624	855.645	0.38
IW (4.3V)	853.417	855.604	0.193

Sample	Ni^{2+} (853.3 eV)	Ni^{3+} (855.0 eV)	Ni^{4+} (856.6 eV)
NMC622 (fresh)	56%	44%	N/A
IW (fresh)	56%	44%	N/A
NMC622 (4.3V)	27%	N/A	73%
IW (4.3V)	16%	N/A	84%

Cell potential	NMC622	with additive
OCV (3.0V)	I_{003}/ I_{104} = 1.888	I_{003}/ I_{104} = 1.861
4.3 V	I_{003}/ I_{104} = 1.564	I_{003}/ I_{104} = 1.601

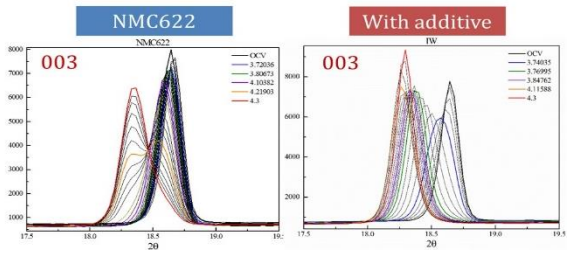


Figure 1. The in-situ electrochemical hard XAS result of Ni XANES, decrease the Ni(II) (Peak A) ratio at 100% SOC.

Figure 2. Preventing cation mixing problem with additive, fully charged NMC622 is unstable with lower I_{003}/ I_{104} ratio.

References

[1] Fu-Ming Wang, J. Membrane Sci. 368 (2014) 165.
[2] Sunny Hy, J. Am. Chem. Soc. 136 (2014) 999.
[3] M.-H. Lin et al. Journal of Power Sources 359 (2017)