

Mechanistic Insight of NCM Cathode in Li ion Battery

Hung-Ling Yu (游鴻霖)^{1*}, Sheng-Yu Yu (游聲宇)¹, Kassa-Belay Ibrahim¹,
Mau-Tsu Tang(湯茂竹)², Chih-Wen Pao(包志文)², and Heng-Liang Wu(吳恆良)¹

¹ Center for Condensed Matter Sciences, National Taiwan University, Taipei 10617, Taiwan

² National Synchrotron Radiation Research Center, Hsinchu, Taiwan

hunglingyu1994@gmail.com

Abstract

The capacity and stability of cathode material is the key for development of lithium ion battery. Although NCM Layered oxide ($\text{LiNi}_{0.x}\text{Co}_{0.y}\text{Mn}_{0.z}\text{O}_2$, abbreviated as NCM $x:y:z$) cathode with high Ni content ($x > 0.5$) shows high capacity, the low cyclability and instability at high potential ($>4.25\text{V}$ vs Li/Li^+) is still a major obstacle for the commercialization. In order to improve the performance of high Ni content NCM cathode, the detailed reaction mechanism is highly needed. In this study, the charge compensation mechanism and local structure of NCM were investigated with in-situ X-ray absorption spectroscopy (XAS). The reaction homogeneity was probed by nanoprobe XAS. The oxidation state of Ni increases from 2+ to 4+, while the oxidation state for Co and Mn has minimum variation during the charge process. The Ni-O bond decreases at $\sim 4.25\text{V}$ which could be associated with the drastic decrease of the lattice constant. The XAS results show that the changes in oxidation state of Ni are associated with the capacity, while Mn keeps the structure stable. Nanoprobe XAS mapping results show that the electrochemical reaction is not homogeneous on the particle. In conclusion, the charge is mainly compensated by the oxidation and reduction of Ni during the charge and discharge process. The highly oxidized Ni could cause the lattice contraction, while the Mn is not further oxidized during charging.