Study of Doping Effect on the Cyclability of $LiNi_{0.5}Mn_{1.5}O_{4-\delta}$ Cycled Between 5.0V and 1.0V Using In Situ Synchrotron X-Ray Diffraction

Jaesang Yoon[a], Taewhan Kim[a], Woosung Choi[a], Soyeong Yun[a], Hyunwoo Kim[a], Hyunyoung Park[a], Won-sub Yoon[a,*]

[a] *Department of Energy Science, Sungkyunkwan University, Suwon 16419, South Korea*

E-mail: jaesangs@skku.edu

Zr-doped $LiNi_{0.5}Mn_{1.5}O_4$ (Zr-LNMO) is synthesized by a solid-state method and the effects of Zr-doping on its structural behavior are systematically investigated by using synchrotron-based *in situ* x-ray diffraction during the 1st and the 2nd cycles between 1.0 and 5.0 V. Differences in the structural changes for Zr-LNMO and LNMO during cycling were clearly observed. Both samples show similar reversible phase transitions between three cubic phases and two tetragonal phases during the 1st cycle. However, during the 2nd cycle, overall phase transitions between tetragonal and cubic phases for Zr-LNMO show more reversible features than those for LNMO. *In situ* XRD results during the 2nd cycle reveal that some parts of LNMO cathode materials do not contribute to the capacity, due to the incomplete phase transition between cubic and tetragonal phases and sluggish phase transition kinetics. It is proposed that the increase in the lattice volume by Zr-doping allows more reversible structural changes during repeated cycling, compared to the undoped LNMO, resulting in the improved capacity retention of Zr-LNMO. This study shows that Zr-doping has a great potential, if optimized, to provide structural stability during repeated cycling, thereby leading to superior cycling stability. More details will be discussed in the meeting.