ABSTRACT

In the present work, first the process parameters are optimized to synthesize lithium nickel cobalt oxide solid solution cathodes to yield high discharge capacity and rate capability with decent capacity retention upon repeated charge discharge cycling in the voltage range of 3.0 to 4.2 V. The cyleability has been found to be markedly improved in zirconium modified solid solutions. X-ray Rietveld refinement in conjunction with X-ray photoelectron spectroscopy and micro-Raman spectroscopic analyses have been performed to understand the effect of cation doping in improving the electrochemical characteristics of the synthesized cathode materials. Using a solution based synthesis route, $Li(Li_{1/3}Mn_{2/3})O_2$ in different weight proportions are structurally integrated into the zirconium modified lithium nickel cobalt oxide solid solution. The synthesized cathodes have been characterized systematically in terms of their phase formation behavior, microstructure evolution and electrochemical characteristics. The global structure of the pristine cathodes is characterized using Rietveld structural refinement of the X-ray diffraction patterns. To gain insight about the nature of the structural integration between $Li[Li_{1/3}Mn_{/2/3}]O_2$ and zirconium modified nickel oxide solid solutions, micro-Raman spectroscopy and high-resolution transmission electron microscopy measurements are performed on the pristine cathode particles. The galvanostatic charge-discharge characteristics of these cathodes are investigated in different cut-off voltage windows. X-ray photoelectron spectroscopy analyses of the valence states of the constituent elements are performed in virgin, fully charged and discharge states of selected cathodes. These analyses help us to understand the lithium ion intercalation behavior in these cathode materials. Guided by the analyses of these experimental results we have successfully synthesized high capacity $Li(Li_{1/3}Mn_{2/3})O_2$-$Li(Ni,Co,Mn)O_2$ based cathodes with excellent electrochemical characteristics.

Key words: High energy density cathode, Doping, Solid solution/composite cathode, Rietveld refinement, XPS, Raman spectroscopy, Micrographs, etc.