In-situ X-ray diffraction studies of abused LiMn₂O₄-LiNi_{1/3}Co_{1/3}Mn_{1/3}O₂ composite cathode materials in Li-ion batteries

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Recently, the lithium ion batteries have been investigated intensively and widely used in energy devices and storage systems. For the lithium ion battery applications, LiMn₂O₄ spinel have been investigated as one of the promising material for conventional cathode due to its low cost, low toxicity, fast kinetics and remarkable safety properties.¹ The new layered LiNi_{1/3}Co_{1/3}Mn_{1/3}O₂ cathode material is another good candidate due to its low cost, high specific capacity, and good thermal stability properties.² There are many reports about thermal properties of $LiMn_2O_4$ and $LiNi_{1/3}Co_{1/3}Mn_{1/3}O_2$ cathode material using various techniques such as differential scanning calorimetry (DSC), thermogravimetry/differential thermal analysis (TG/DTA), accelerated rate calorimetry (ARC), and micro-calorimetry.^{3,4} However, not much information on the structural changes of over-charged or over-discharged $LiMn_2O_4$ and $LiNi_{1/3}Co_{1/3}Mn_{1/3}O_2$ cathode has been reported. In the case of $LiNi_{1/3}Co_{1/3}Mn_{1/3}O_2$ cathode materials, at over-charged states (highly delithiated), the reduction of Ni⁴⁺ releases oxygen that can accelerate severe thermal runaway by reacting with the electrolyte before leading to catastrophic failure of the battery.⁵

In this paper, the results of the structural change studies of the over-charged or over-discharged $LiMn_2O_4$ - $LiNi_{1/3}Co_{1/3}Mn_{1/3}O_2$ composite cathode during cycling using in situ synchrotron based XRD technique are reported. These results provide valuable guidance for the structural change behavior and different contributions of each individual component. Additionally, helpful information in redesigning and optimizing the $LiMn_2O_4$ and $LiNi_{1/3}Co_{1/3}Mn_{1/3}O_2$ composite cathode will be provided for Li-ion battery research.

Detailed the electrochemical and structural properties of $LiMn_2O_4$ - $LiNi_{1/3}Co_{1/3}Mn_{1/3}O_2$ composite cathode will be presented at the meeting.

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