Stablilty of $Li[Ni_{0.5}Mn_{0.5}]O_2$ Cathode Compound Synthesized by a Sol-gel Process Investigated by In-situ X-ray Diffraction Analysis

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Due to their low cost and improved stability, $Li[Ni_{0.5}Mn_{0.5}]O_2$– based materials are considered possible alternatives to $LiCoO_2$- and $LiNiO_2$- based cathode matrials for rechargeable lithium batteries. The material $Li[Ni_{0.5}Mn_{0.5}]O_2$ shows stable reversible capacity up to 200 mAh/g in the potential window of 2.5-4.5 V. The sepration of Li and transition metals in different layers is not perfact in $Li[Ni_{0.5}Mn_{0.5}]O_2$ as Rietveld refinement of the structure based on XRD and neutron diffraction data gives 8-10% Ni ions in the Li layer. Such mixing is naturally accompanied by the presence of Li ions in the transition metal layers, which has been revealed by Li magic angle spinning NMR studies. Hence, the cation mixing of the electrode structure is concerned with stability. Thus, we have performed in-situ X-ray diffraction (XRD) measurements of $Li[Ni_{0.5}Mn_{0.5}]O_2$ during charging process using the high energy beam at 01C2. The cathode material is prepared by a sol-gel process and cell is tested in the potentials from OCP(2.939) ~to 5.828 V at 0.1C. The in-situ X-ray diffraction pattern shows that the well defined (003) peak and the splitting of (106), (221), (108) and (110) reflections are clearly, indicating that the synthesized material has layer characteristics and the peak indexing is done based on the α-$NaFeO_2$ structure. The diffraction peak shift to the higher angles indicates the decrease in the lattice parameter in the lattice. The peak positions are gradually shifted to higher angles with the extraction of Li ions suggesting that the structure (rhombohedra) gradually transformed to the monoclinic phase. In addition, the diffraction peak positions are not changed in the potential window of 5.110-5.828V indicating that the extraction of lithium ions is probably due to the reaction with electrolyte. In-situ X-ray diffraction (XRD) investigations provide valuable information which can not be obtained by the conventional X-ray diffraction due to the significant difference in the scattering factors of various cations. The structural properties suggest that the $Li[Ni_{0.5}Mn_{0.5}]O_2$ cathode compound is a high stability electrode candidate for advanced lithium-ion batteries.

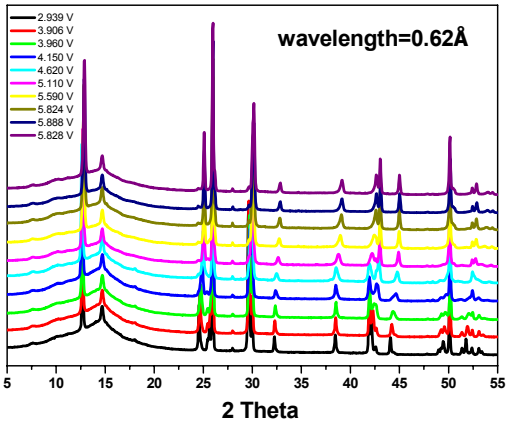

Figure1. In-situ XRD patterns of $Li[Ni_{0.5}Mn_{0.5}]O_2$ during Charge.