Poster

Structural effects from varying the Fe/Mn ratio in layered $NaFe_yMn_{1-y}O_2$ for Na-ion batteries

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Most Li-ion batteries rely on chemistries inclosing toxic and scarce elements such as Co, Ni and Li. Thus, developing novel and sustainable alternative technologies based on abundant elements such as Na, Mn and Fe is of high priority [1, 2]. During recent years sodium ion batteries have greatly improved and become a promising substitute for the current Li-ion technology. Herein the layered transition metal oxides are promising class of electrode material due to their high capacity. However, we still lack to identify materials with truly sustainable elemental compositions, which provides stable capacities with repeated dis-/charge of the battery. Materials based on iron and manganese, $NaFe_yMn_{1-y}O_2$ are of high interest due to the high abundance of these elements and reports have shown capacities exceeding 160 mAh/g [3-5]. The layered transition metal oxides are typically obtained in one of two polymorphs denoted as the P2- or O3-phase. The O3-phase is interesting due to a higher initial sodium loading, i.e. higher capacity, compared to P2-analogoues.

In this study, we investigate how the structural phase transitions are affected by varying the Fe:Mn ratio in O3-$NaFe_yMn_{1-y}O_2$ (y = 0.5, 0.6, 0.7 and 0.8). The materials with high Fe-content, $NaFe_{0.7}Mn_{0.3}O_2$ and $NaFe_{0.8}Mn_{0.2}O_2$, transform via second order phase transitions into an unknown O3-like phase upon Na intercalation, while samples with low Fe content, $NaFe_{0.5}Mn_{0.5}O_2$ and $NaFe_{0.6}Mn_{0.4}O_2$, go through multiple phase transitions involving (figure 1). Interesting, the first and second charge differs in $NaFe_{0.5}Mn_{0.5}O_2$, where an unidentified “X-phase” forms due to severe stacking faults during the second cycle. Our analysis of the X-phase shows that it bears a closer resemblance to an O3-state than a P3-state, suggesting a higher probability of finding an octahedral layer compared to prismatic Na coordination.

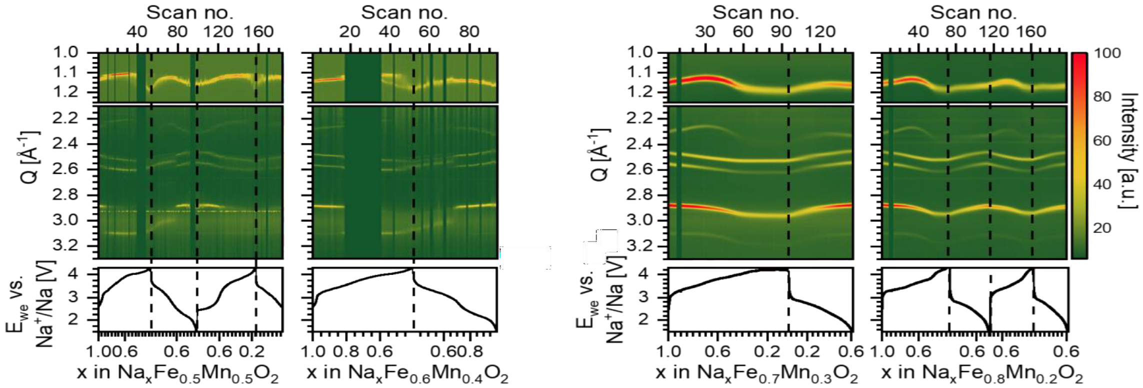

Figure 1. Powder X-ray diffraction overview plots (top) as a function of electrochemical performance in $NaFe_xMn_{1-x}O_2$ (x = 0.5, 0.6, 0.7 and 0.8) from left to right. The structural diversity for $NaFe_{0.5}Mn_{0.5}O_2$ and $NaFe_{0.6}Mn_{0.4}O_2$ appear richer compared to the samples with a higher Fe content, $NaFe_{0.7}Mn_{0.3}O_2$ and $NaFe_{0.8}Mn_{0.2}O_2$.

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