Characterization and Electrochemical Performance of Substituted $LiNi_{0.4}Co_{0.2-y}Al_yMn_{0.4}O_2$ ($0 \le y \le 0.2$) Cathode Materials

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Due to the high cost and toxicity of cobalt, a significant amount of research has been directed at developing cathode materials with reduced amounts of this metal. Any new materials must also meet demanding electrochemical performance and safety requirements if they are to be utilized in large-scale applications such as hybrid vehicles. To this end, a new series of aluminum-substituted materials, $LiNi_{0.4}Co_{0.2-y}Al_yMn_{0.4}O_2$ with y ranging from 0 to 0.2, have been synthesized using combustion techniques.[1] Cobalt can be completely substituted with aluminum in this series (Figure 1), consistent with the observed solubility limit of ~0.2-0.35 of other similarly substituted oxide materials[2, 3] crystallizing in the $R\bar{3}m$ space group.

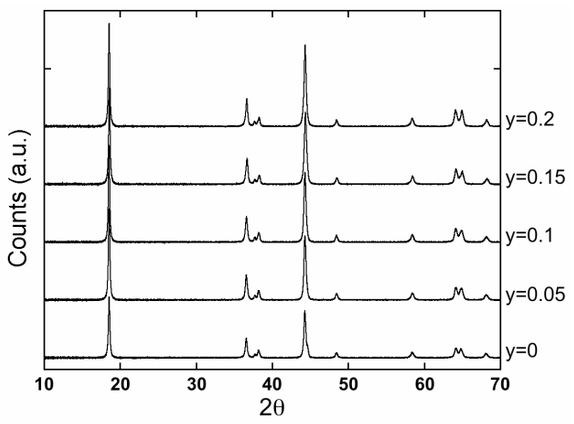

Figure 1. XRD patterns of $LiNi_{0.4}Co_{0.2-y}Al_yMn_{0.4}O_2$ compounds. All peaks can be indexed to the $R\bar{3}m$ space group.

Although the overall theoretical capacity is somewhat reduced upon Al substitution, the main redox process below 4.5V vs. Li is $Ni^{2+} \leftrightarrow Ni^{4+}$.[4] Disregarding Co redox processes, calculated capacities range from 223 mAh/g at y=0 to 239 mAh/g at y=0.2 for the series. Indeed, there appears to be little impact on the practical capacity at low levels of substitution (Figure 2) when charging is limited to 4.3V, and the cycling behavior even appears to be improved somewhat. Furthermore, it is found that at higher current densities (up to 5 mA/cm^2) all of the substituted materials outperform the parent material regardless of the level of substitution.

The thermal characteristics of $LiNi_{0.4}Co_{0.2-y}Al_yMn_{0.4}O_2$ compounds are of paramount interest, considering the increased need for safety and abuse-tolerance in vehicular applications. The presence of Al may ameliorate the effects of the increased Ni content (compared to $LiNi_{1/3}Co_{1/3}Mn_{1/3}O_2$). Thermal characteristics of charged materials will be investigated using TGA, DSC, and *in situ* XRD. The effect of aluminum substitution on the structure (cation distribution) and associated magnetic changes will also be discussed in detail during the presentation.

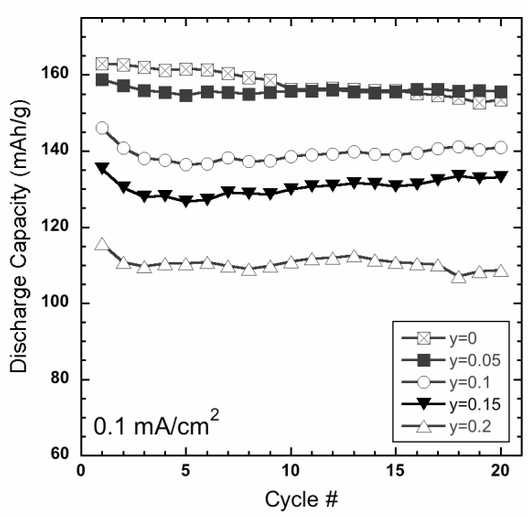

Figure 2: Specific capacities of $LiNi_{0.4}Co_{0.2-y}Al_yMn_{0.4}O_2$ compounds as a function of cycle number (2.0-4.3V).

Acknowledgment

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